Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Ag(I)-Catalyzed Cycloisomerization Reactions: Synthesis of Substituted Phenanthrenes and Naphthothiophenes

Rakesh K. Saunthwal, Abhinandan K. Danodia, Kapil Mohan Saini and Akhilesh K. Verma*

[a]*Synthetic Organic Chemistry Research Laboratory, Department of Chemistry, University of Delhi, Delhi 110007, India*

X-ray crystallographic Study

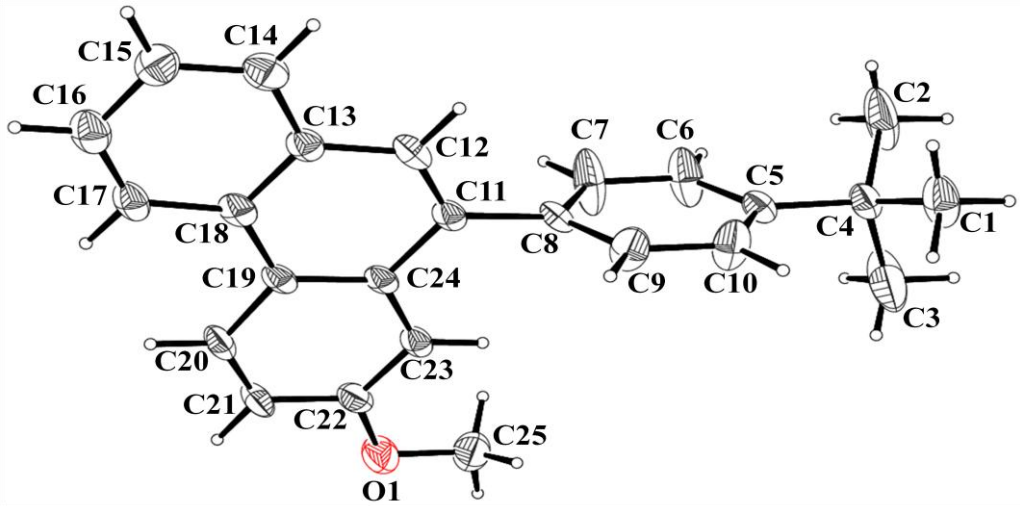


Figure 1. X-Ray Crystallographic Studies.(Thermal ellipsoid are drawn at 30% probability level).

The intensity data for was collected on an Oxford Xcalibur CCD diffractometer equipped with graphite monochromatic Mo-Ka radiation (λ = 0.71073 Å) at 150(2) K[1]. A multi-scan correction was applied. The structure was solved by the direct methods using SIR-92 and refined by full-matrix least-squares refinement techniques on F^2 using SHELXL97[2]. The hydrogen atoms were placed into the calculated positions and included in the last cycles of the refinement. All calculations were done using Wingx software package[3]. CCDC deposit no is 884177

Table 1. Crystal data and structure refinement for 2c.

Empirical formula	C25 H24 O
Formula weight	340.44
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P b c a
A	19.703(2) Å
B	8.2643(5) Å
C	23.1696(19) Å
α	90°
β	90°
γ	90°
Volume	3772.7(6) $Å^3$
Z	8
Density (calculated)	1.199 Mg/m^3
Absorption coefficient	0.071 mm^{-1}
F(000)	1456
Crystal size	0.23 x 0.22 x 0.22 mm^3
Theta range for data collection	3.20 to 25.00°.
Index ranges	$-23 \leq h \leq 22$, $-9 \leq k \leq 9$, $-27 \leq l \leq 22$
Reflections collected	13457
Independent reflections	3315 [R(int) = 0.0469]
Completeness to theta = 25.00°	99.8 %
Absorption correction	Multi-scan
Max. and min. Transmission	0.9845 and 0.9838
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3315 / 0 / 235
Goodness-of-fit on F^2	1.096
Final R indices [I>2sigma(I)][a, b]	R1 = 0.0969, wR2 = 0.2312
R indices (all data)	R1 = 0.1223, wR2 = 0.2465
Largest diff. peak and hole	0.230 and -0.210 $e.Å^{-3}$

[a] $R = \sum(\|Fo\| - \|Fc\|)/\sum|Fo|$; [b] $R_W = \{\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$

References:

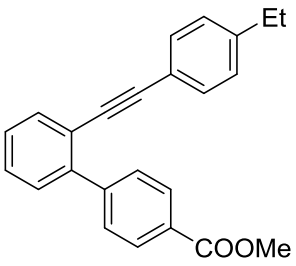
1. CrysAlisPro, Agilent Technologies, Version 1.171.34.49 (**2011**).

2. G. M. Sheldrick, Acta Cryst., **2008**, A64, 112-122.

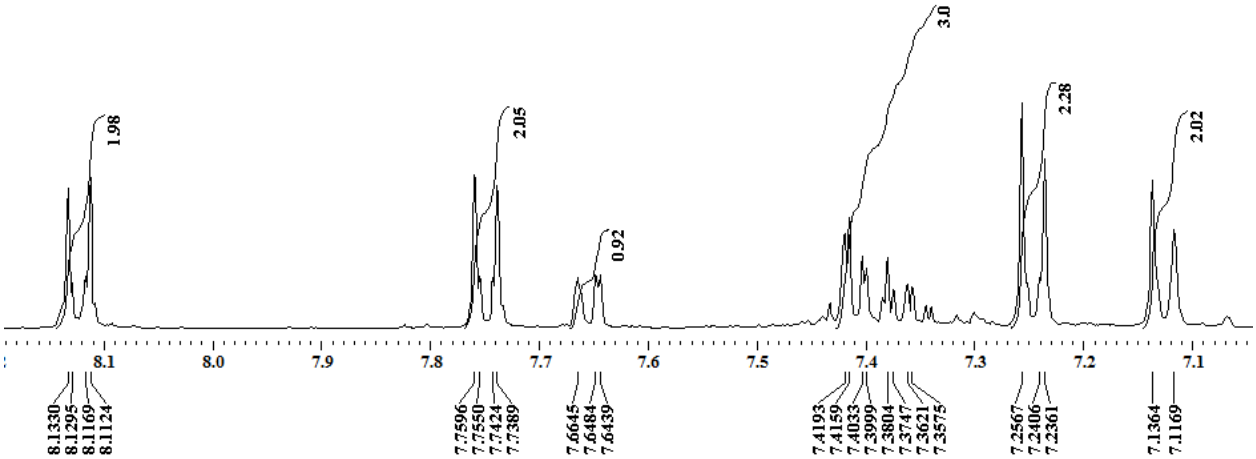
3. L. J. Farrugia, WinGX Version 1.80.05, *An integrated system of Windows Programs for the Solution, Refinement and Analysis of Single Crystal X-Ray Diffraction Data;* Department of Chemistry, University of Glasgow (**1997-2009**).

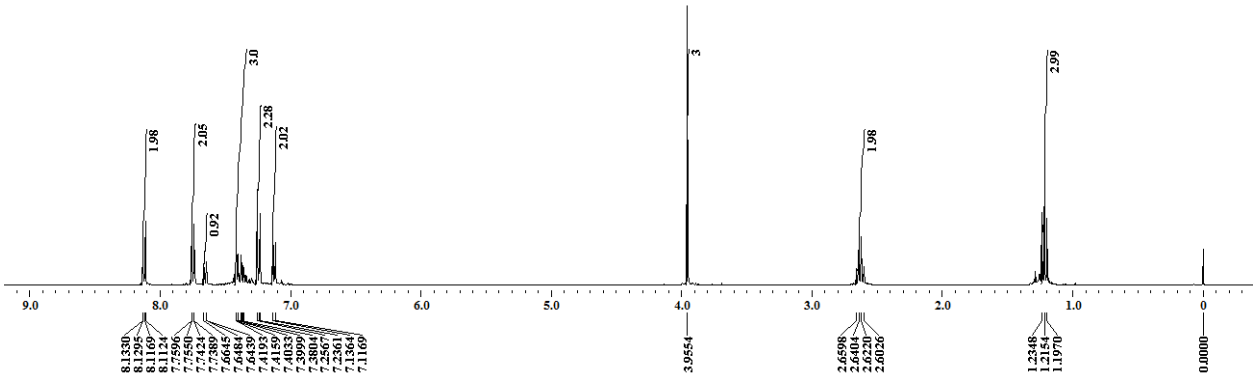
Copies of ^{1}H and ^{13}C NMR

^{1}H NMR

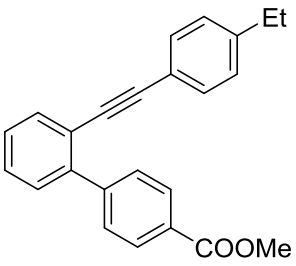


Methyl 2'-((4-ethylphenyl)ethynyl)-[1,1'-biphenyl]-4-carboxylate (1q)

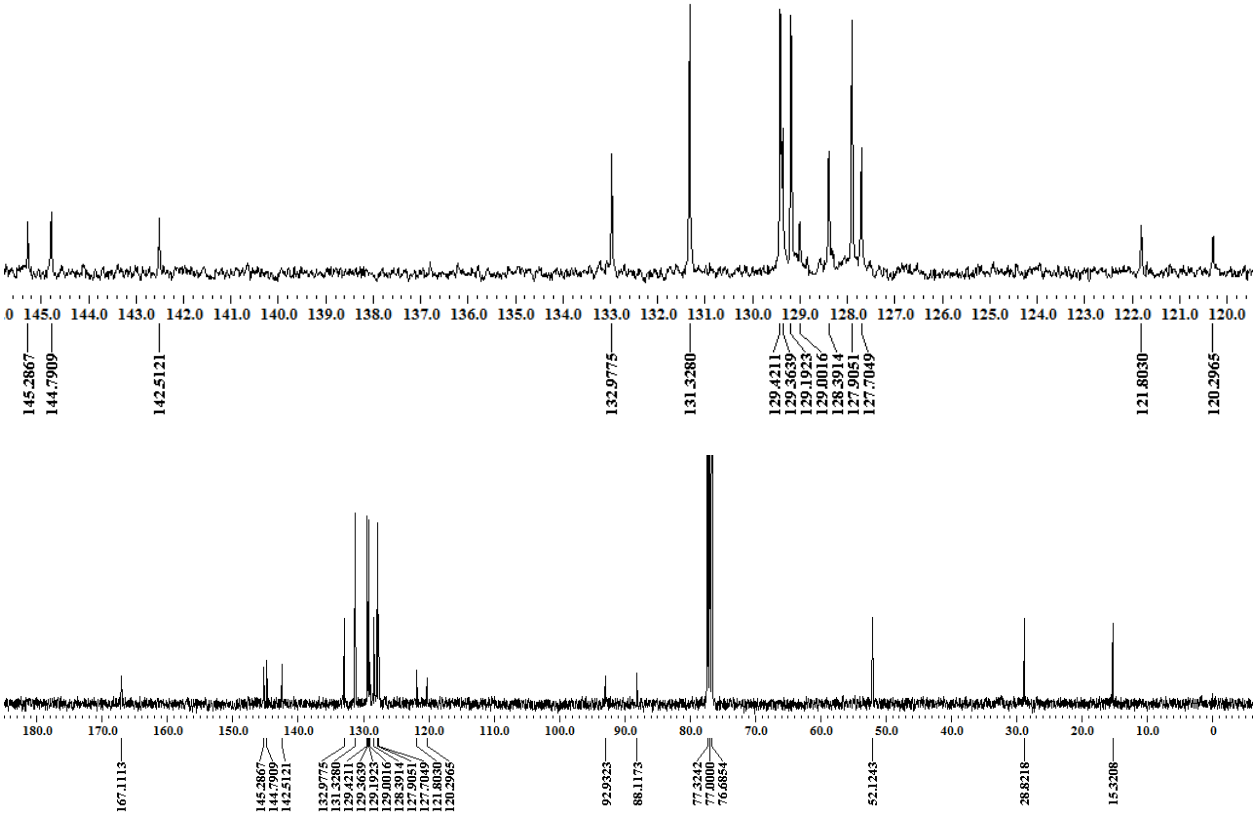




^{13}C NMR



Methyl 2'-((4-ethylphenyl)ethynyl)-[1,1'-biphenyl]-4-carboxylate (1q)



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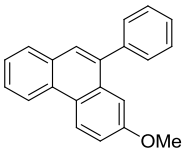
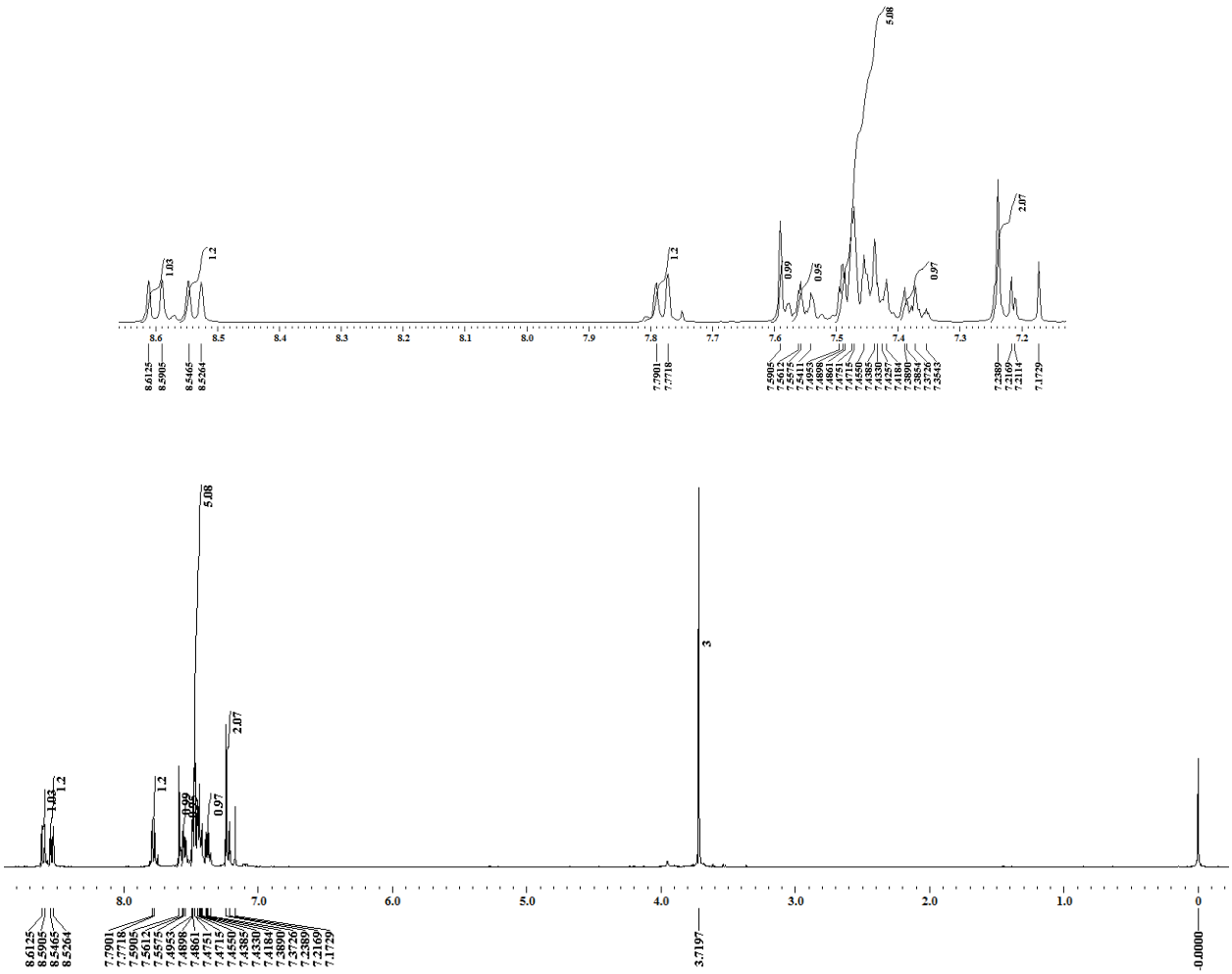


2-Methoxy-10-phenylphenanthrene (2a)



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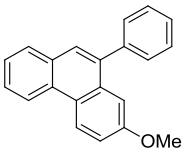

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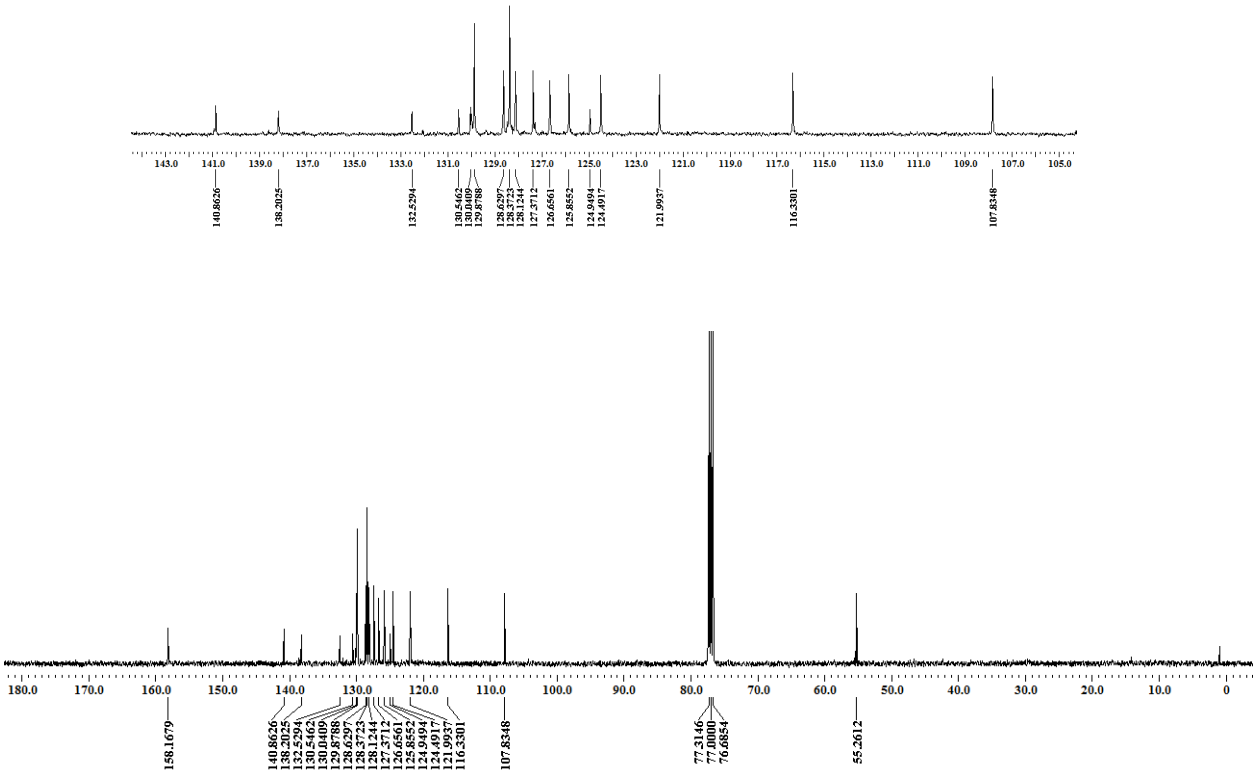

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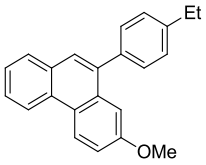

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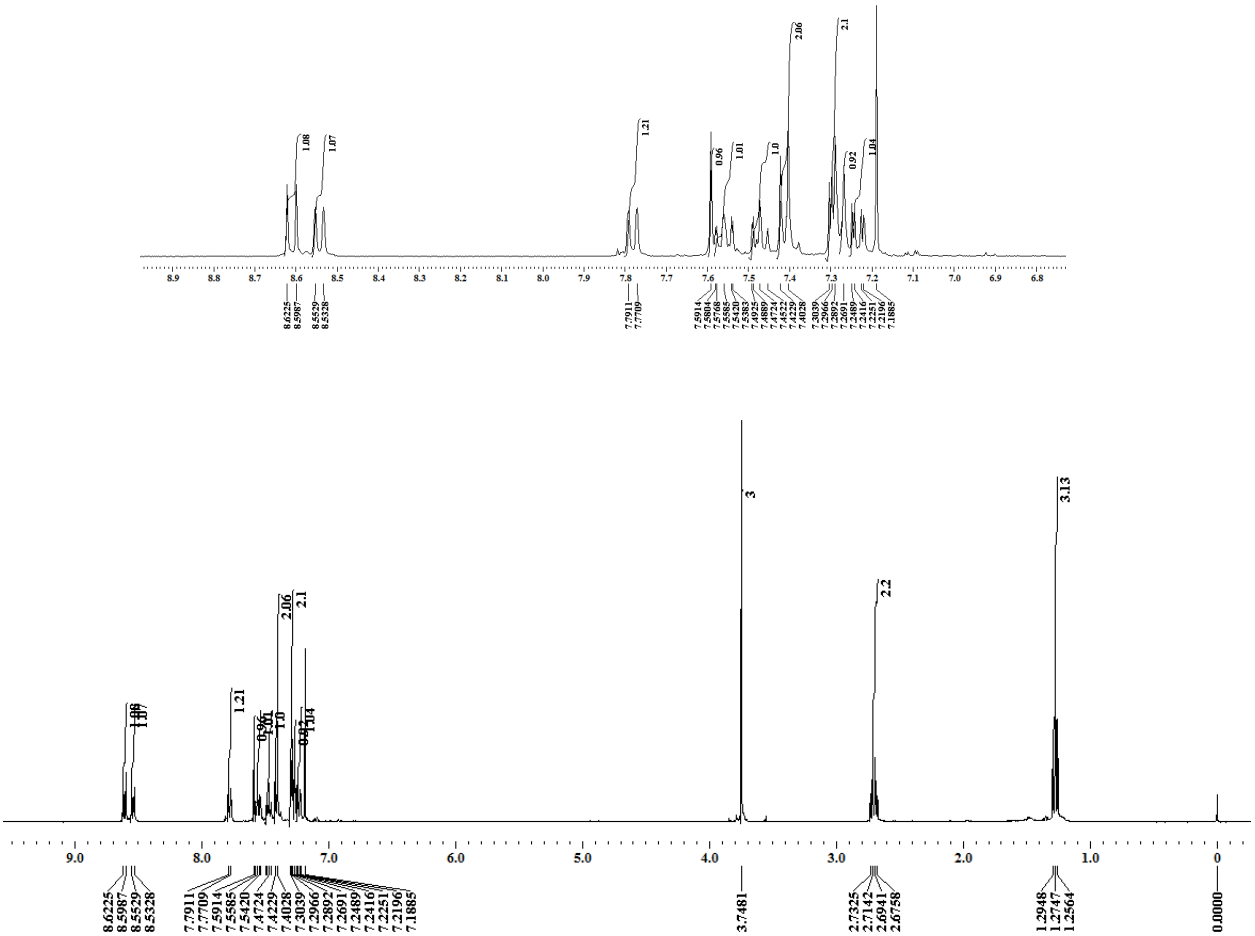

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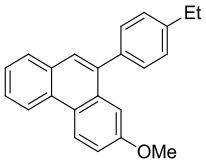
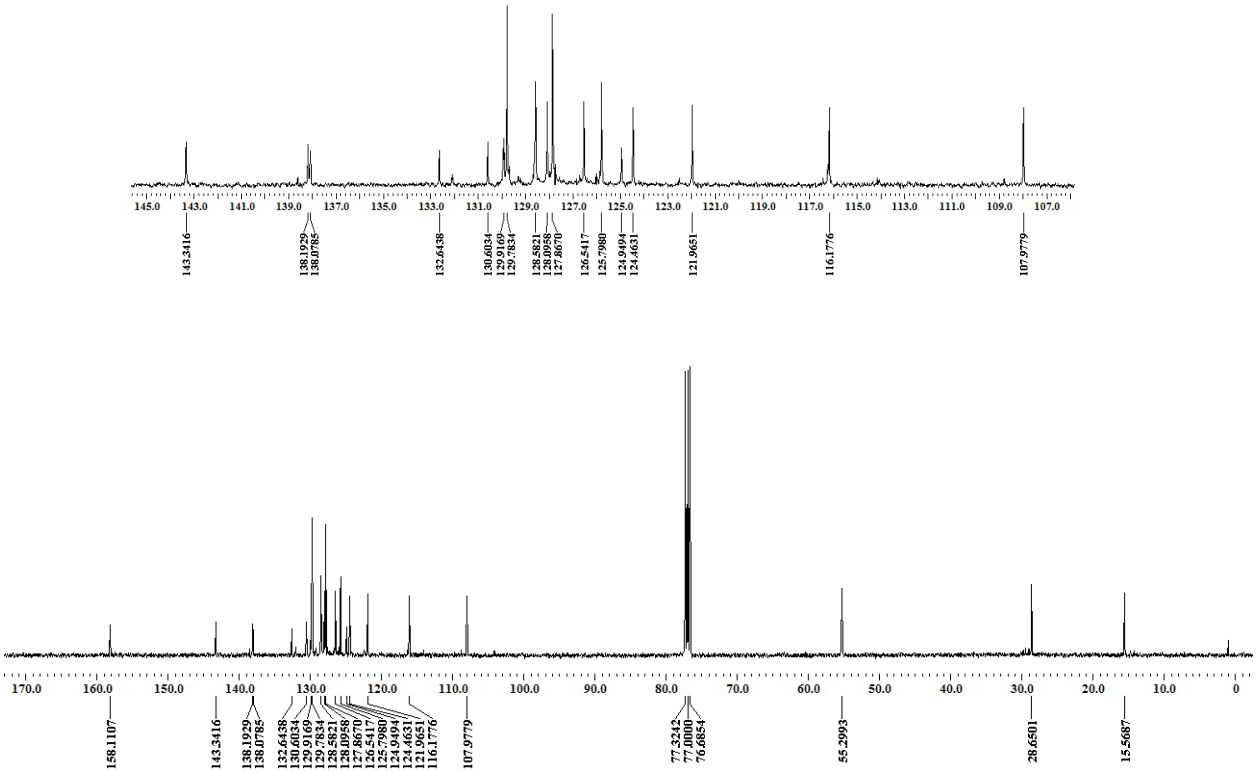


2-Methoxy-10-p-tolyl-phenanthrene (2b)



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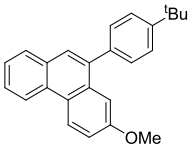

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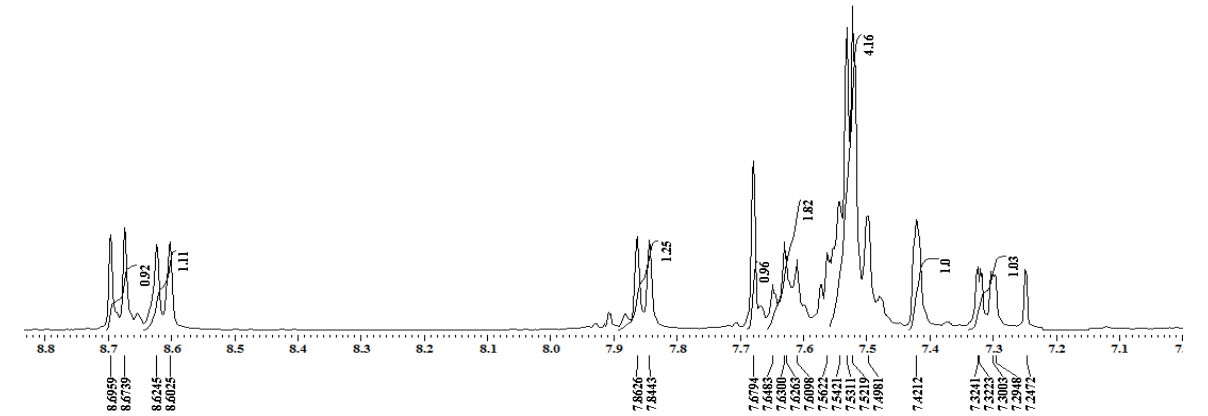

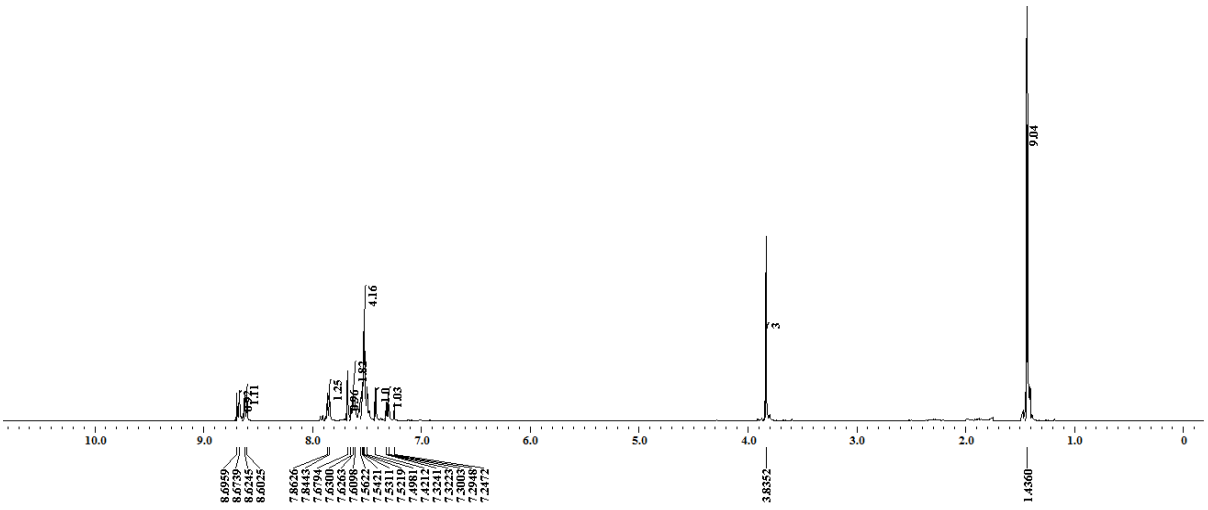

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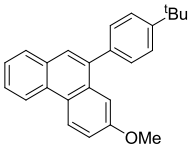

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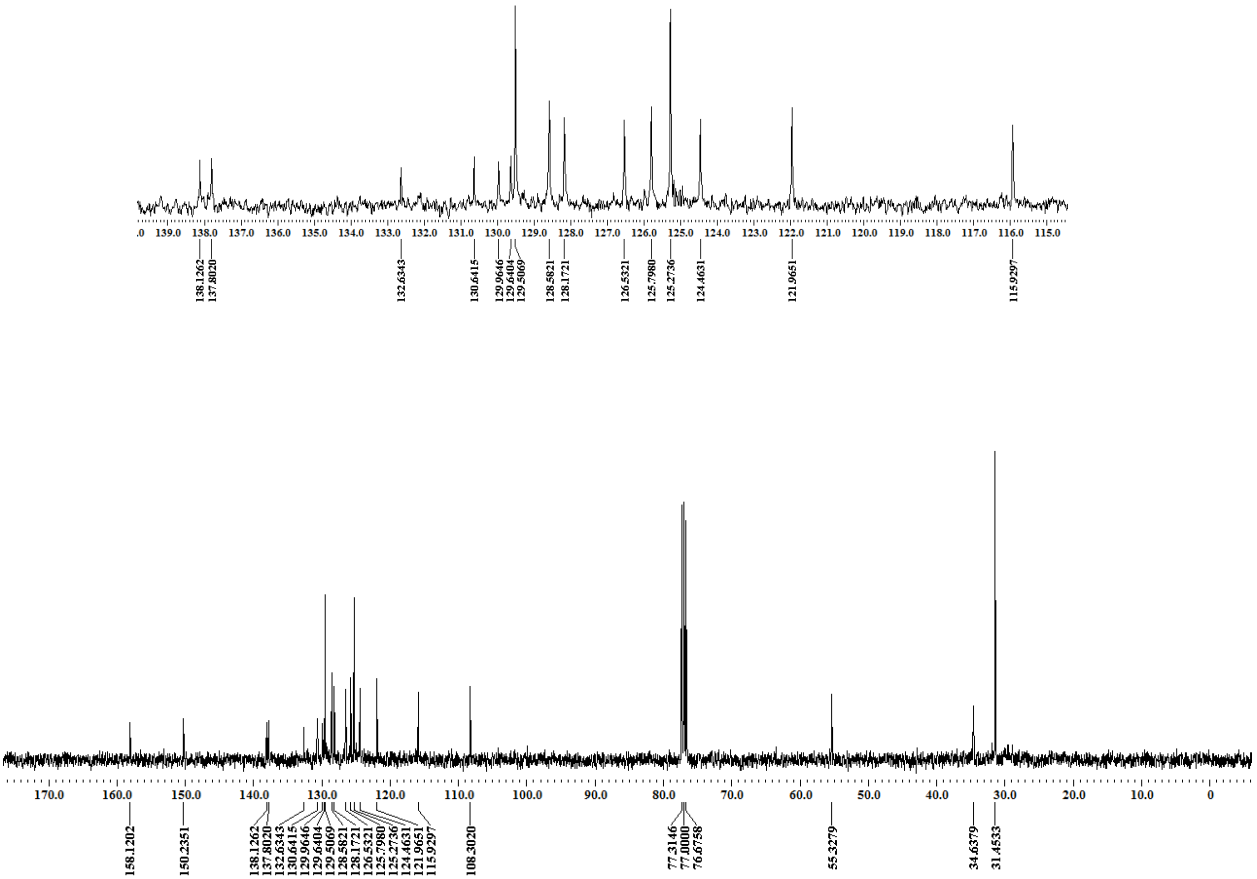

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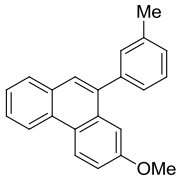

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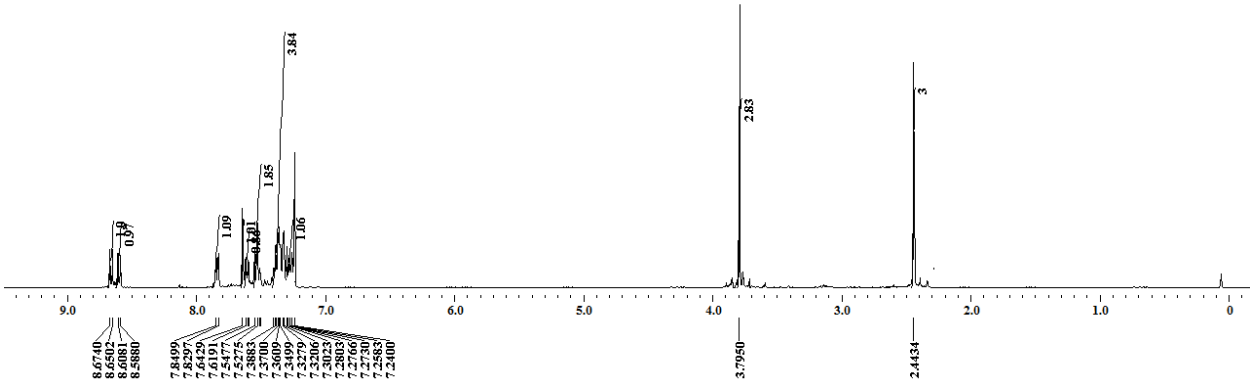

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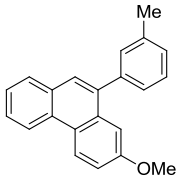

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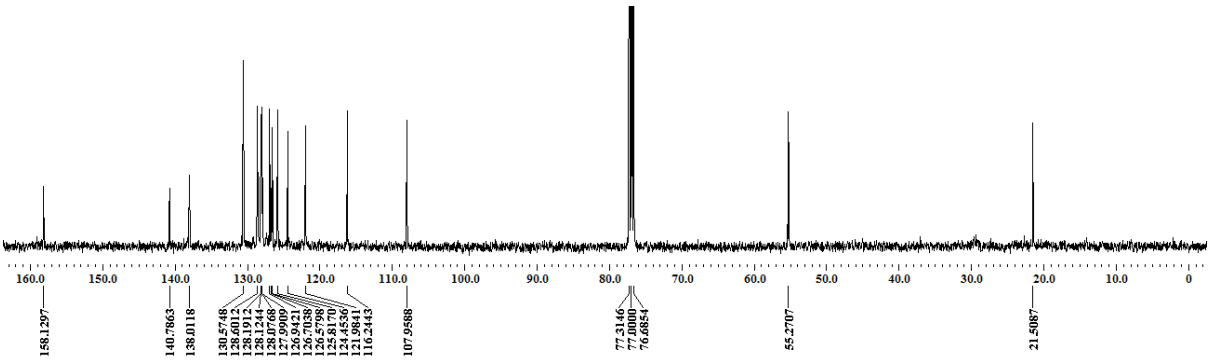

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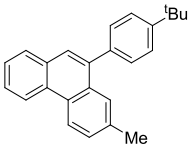

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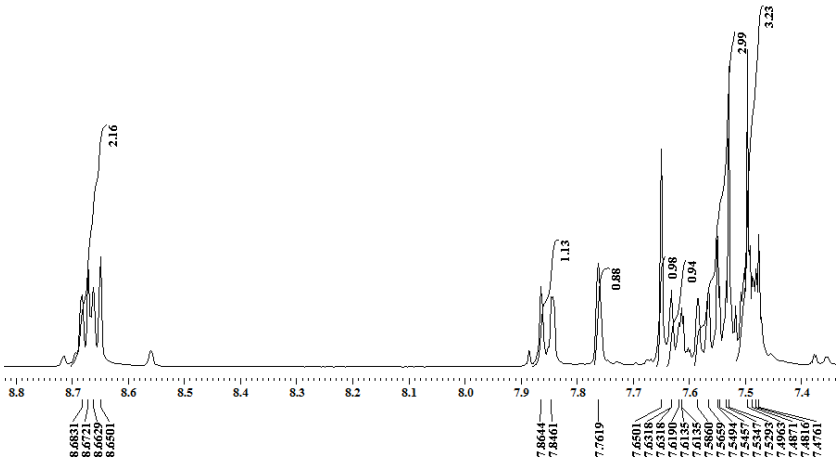

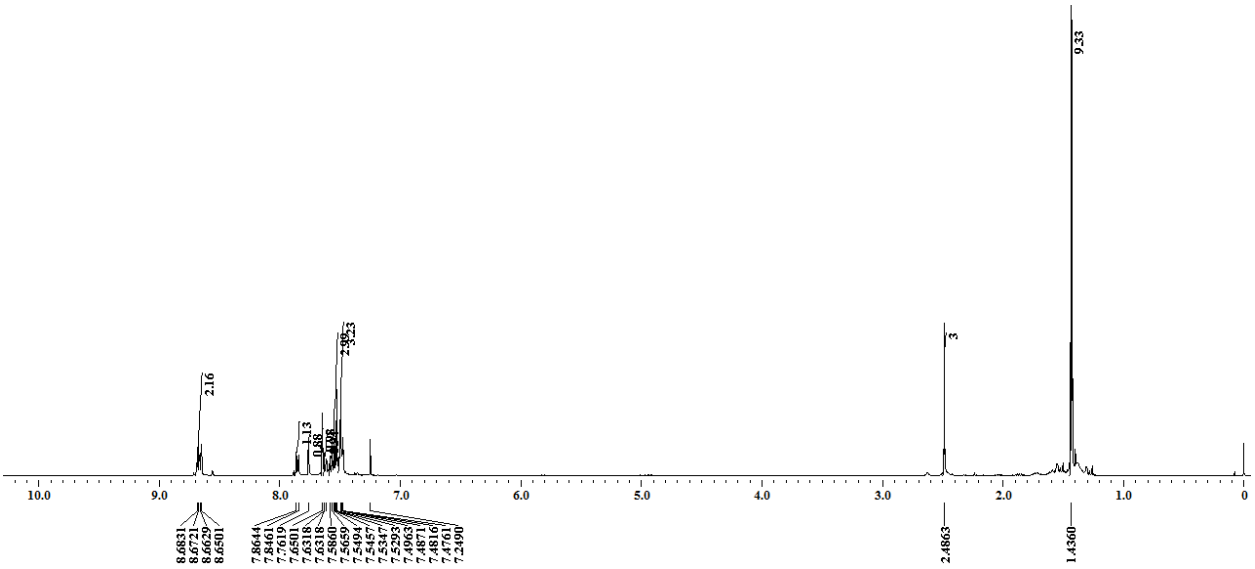

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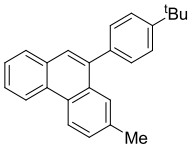

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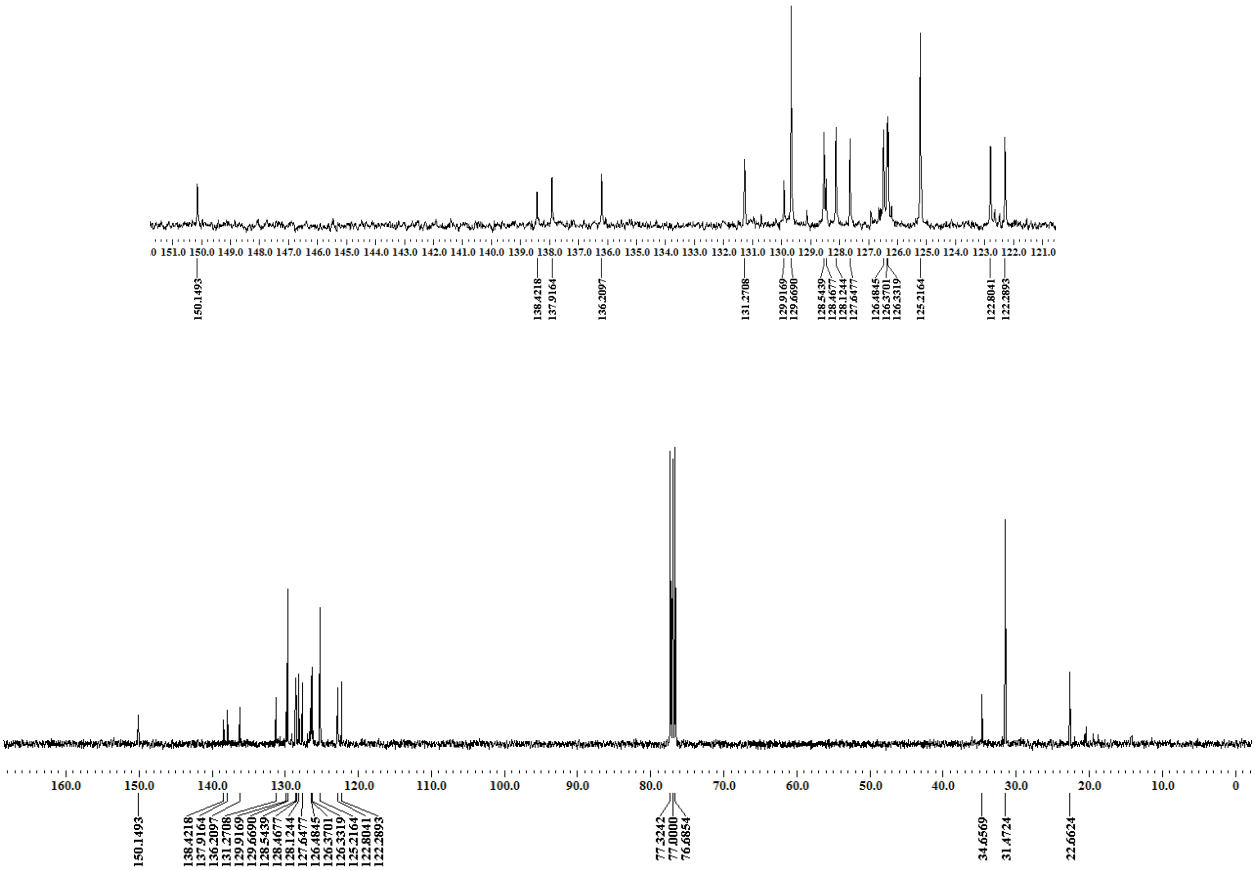

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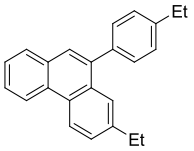

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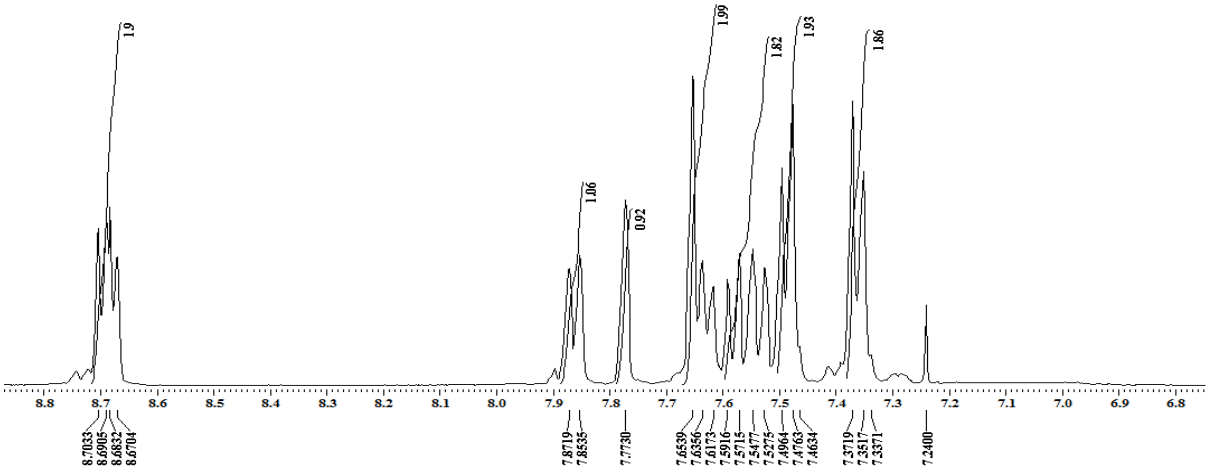

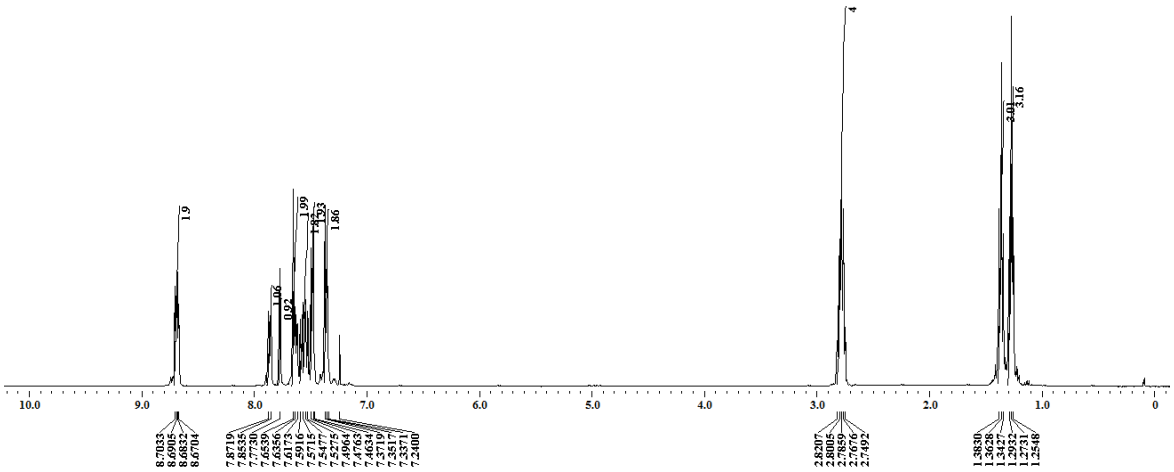

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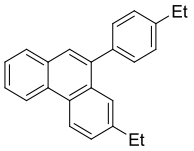
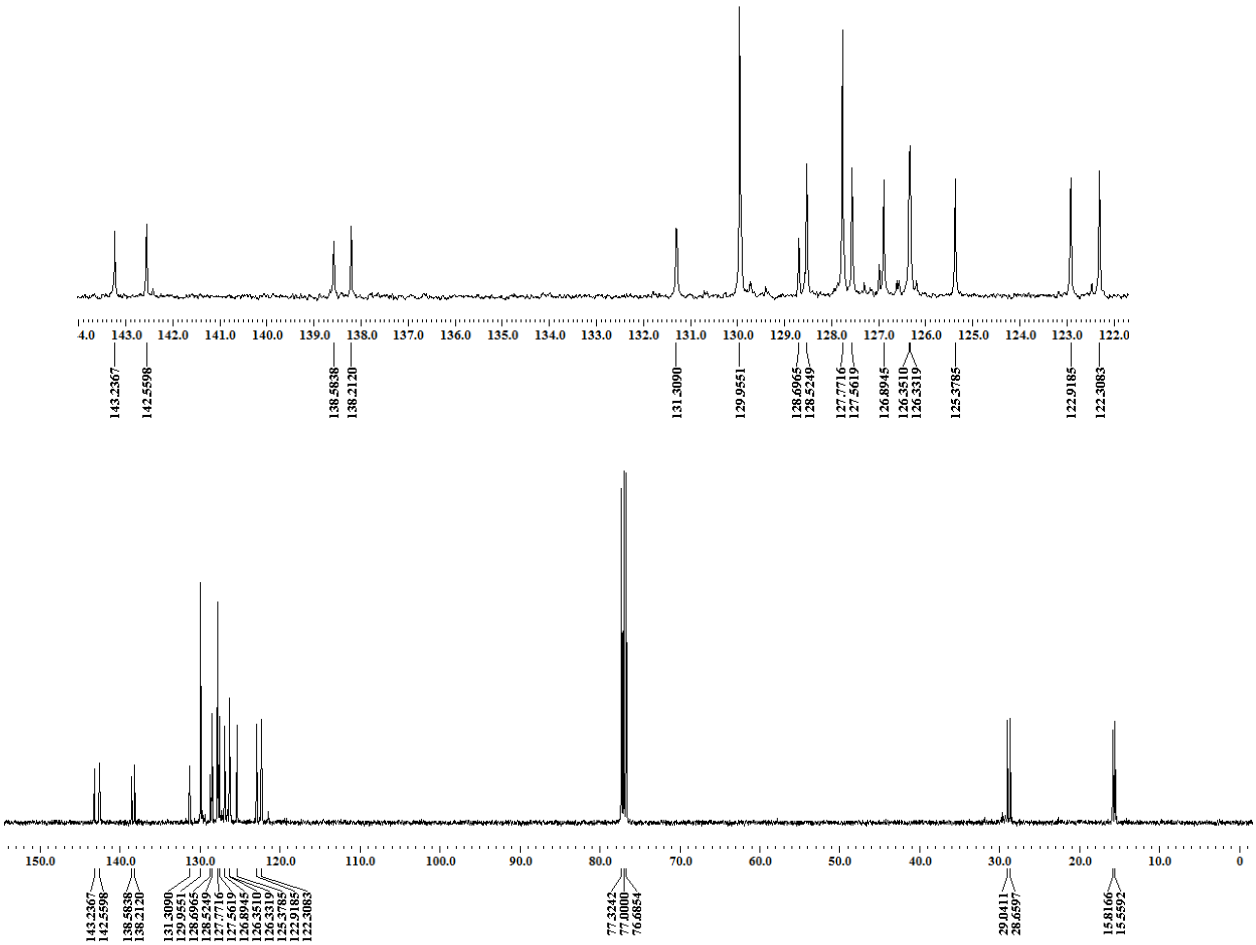


2-Ethyl-10-(4-ethyl-phenyl)-phenanthrene (2f)



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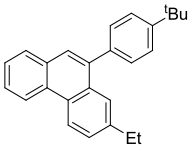

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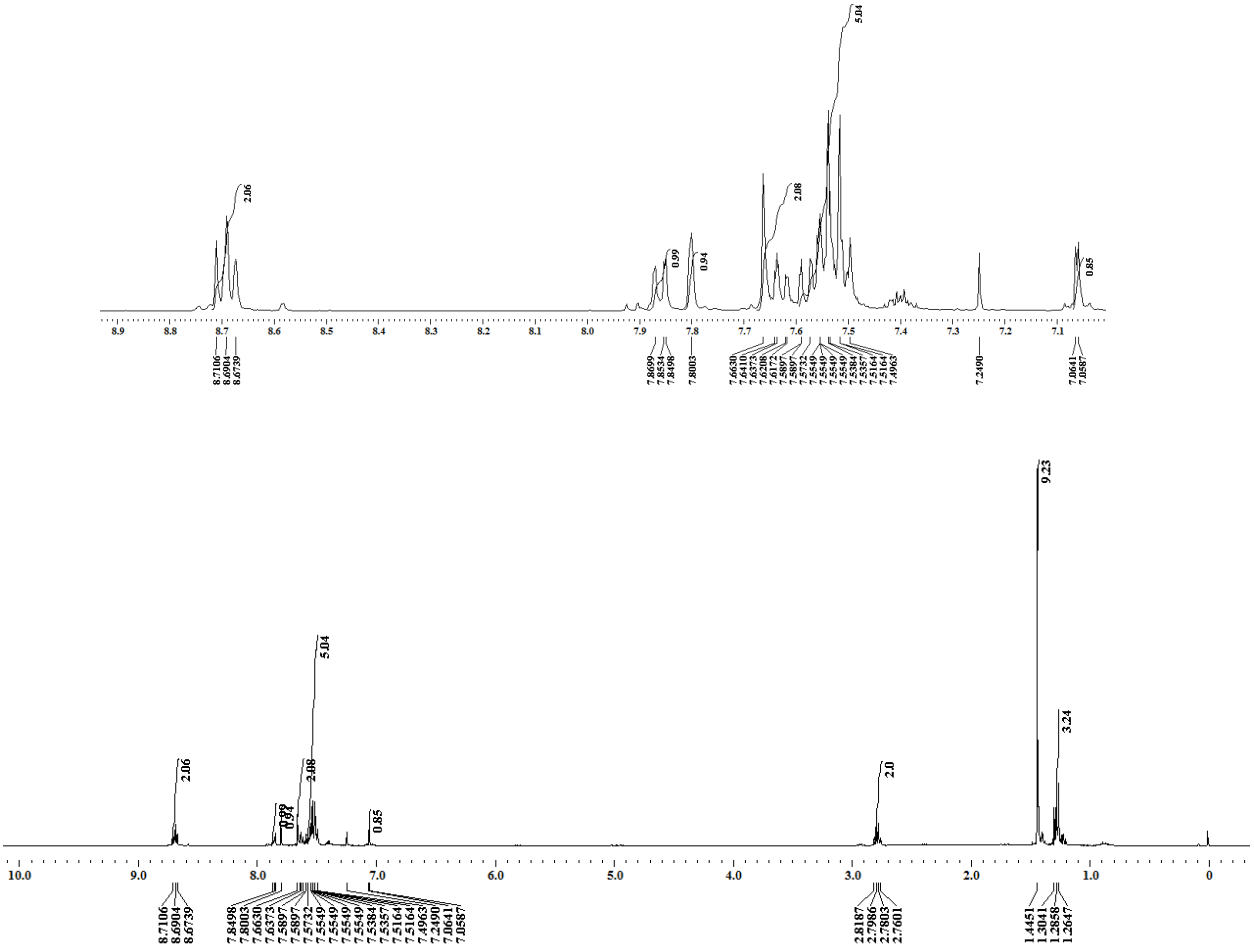

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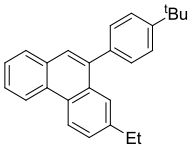
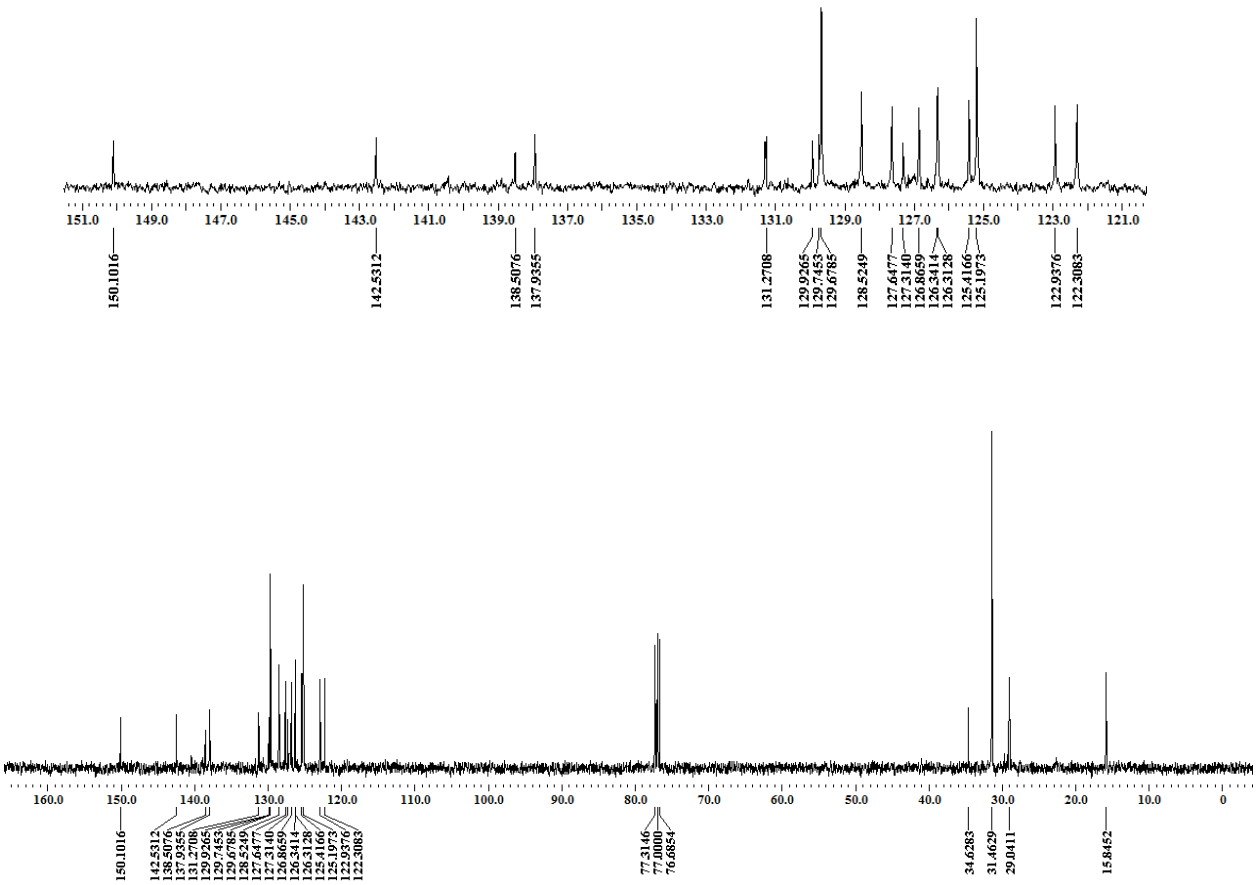


10-(4-*tert*-Butyl-phenyl)-2-ethyl-phenanthrene (2g)



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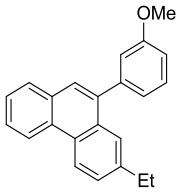
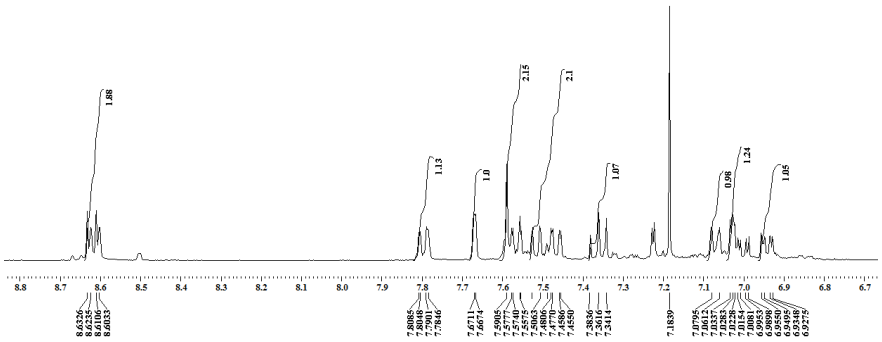
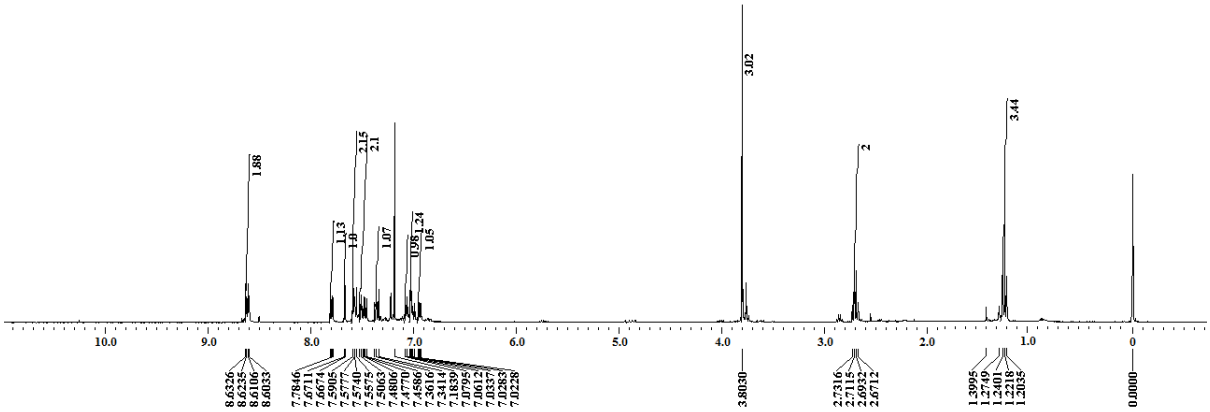


2-ethyl-10-(3-methoxyphenyl)phenanthrene (2h)





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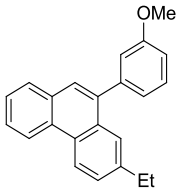
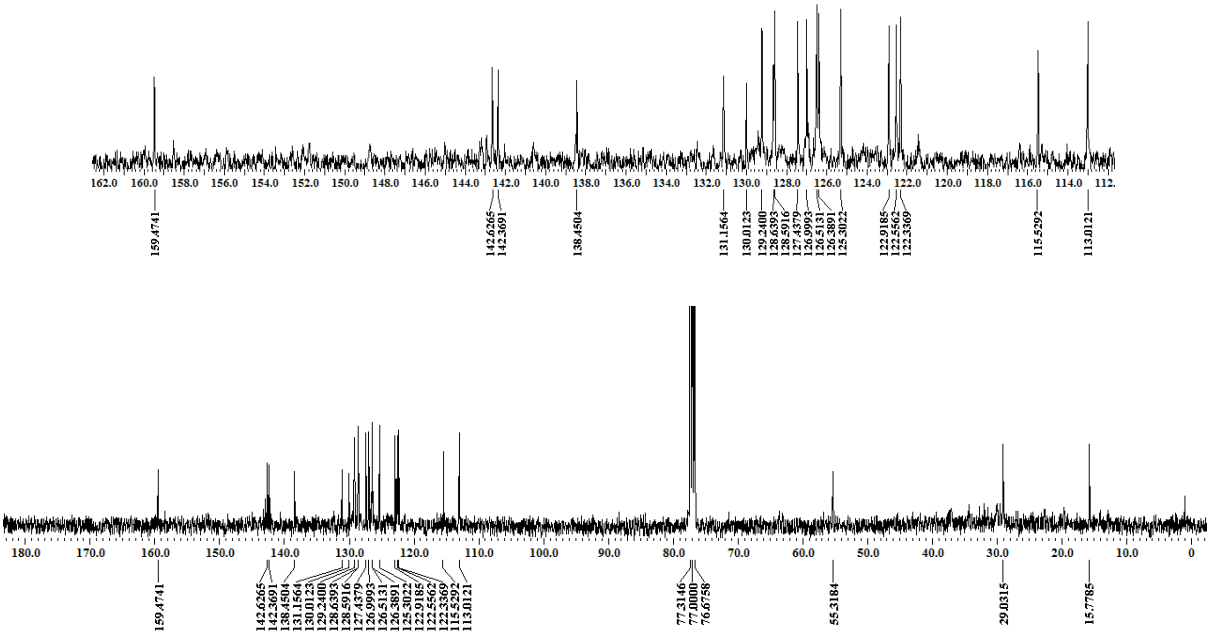


2-ethyl-10-(3-methoxyphenyl)phenanthrene (2h)



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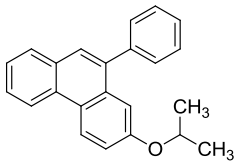
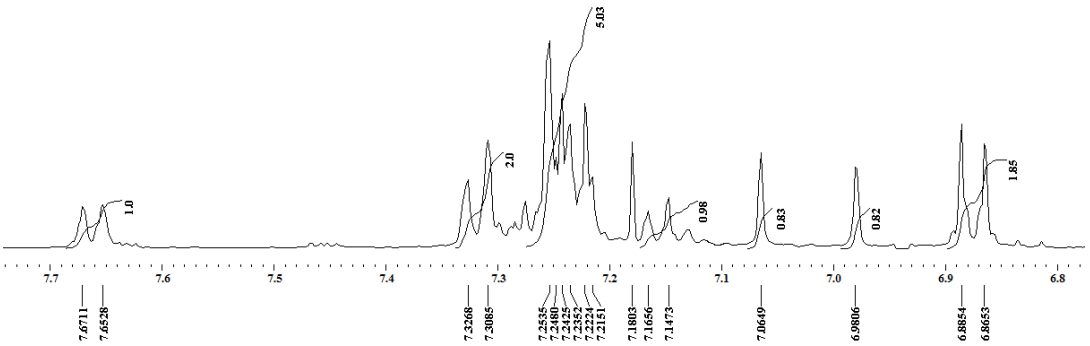
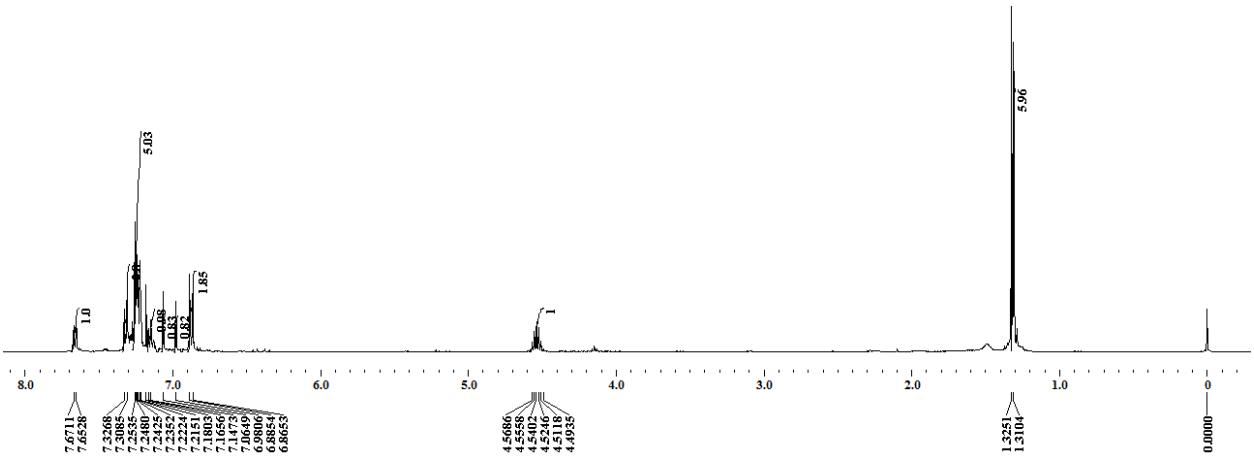


2-Isopropoxy-10-phenylphenanthrene (2i)





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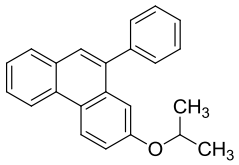

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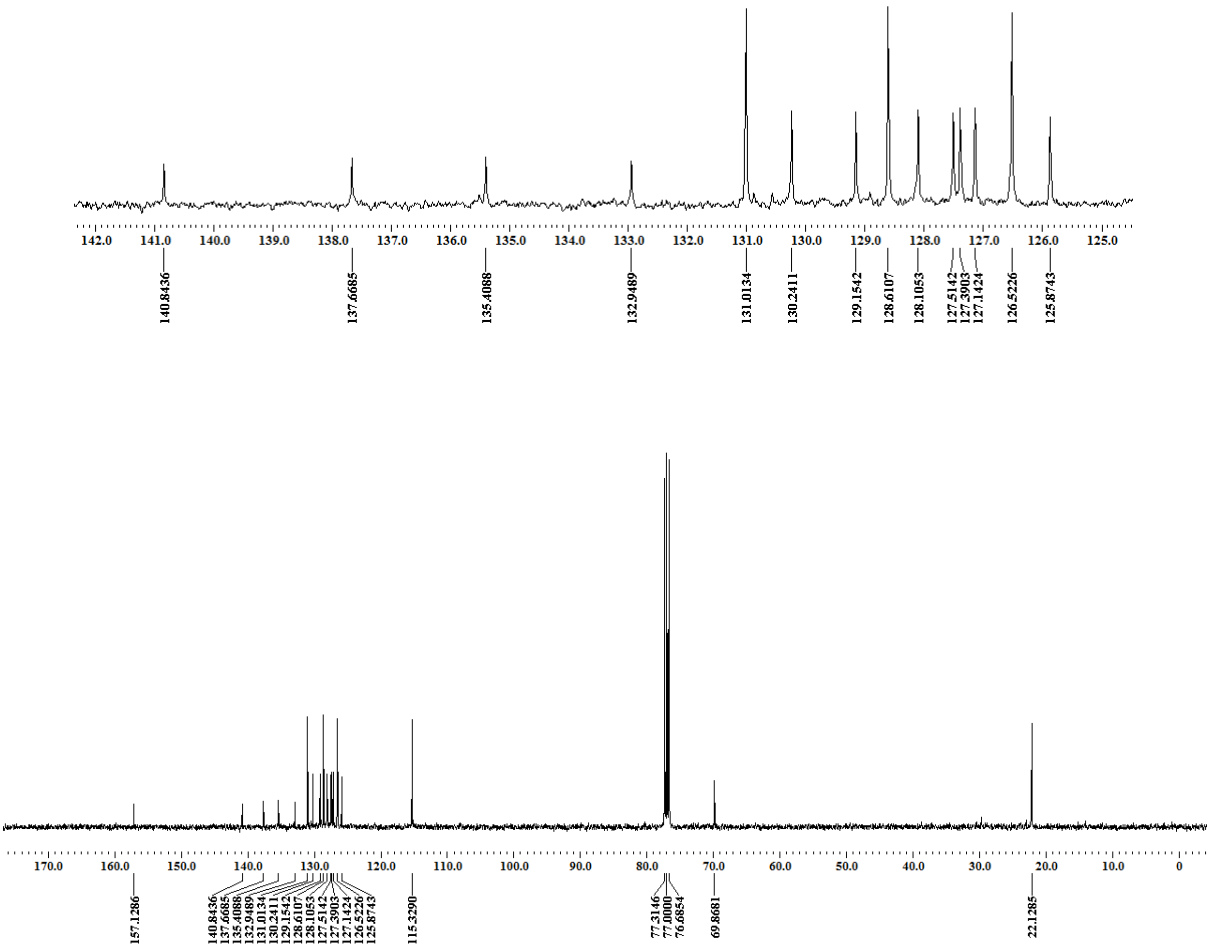

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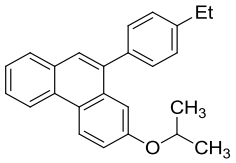

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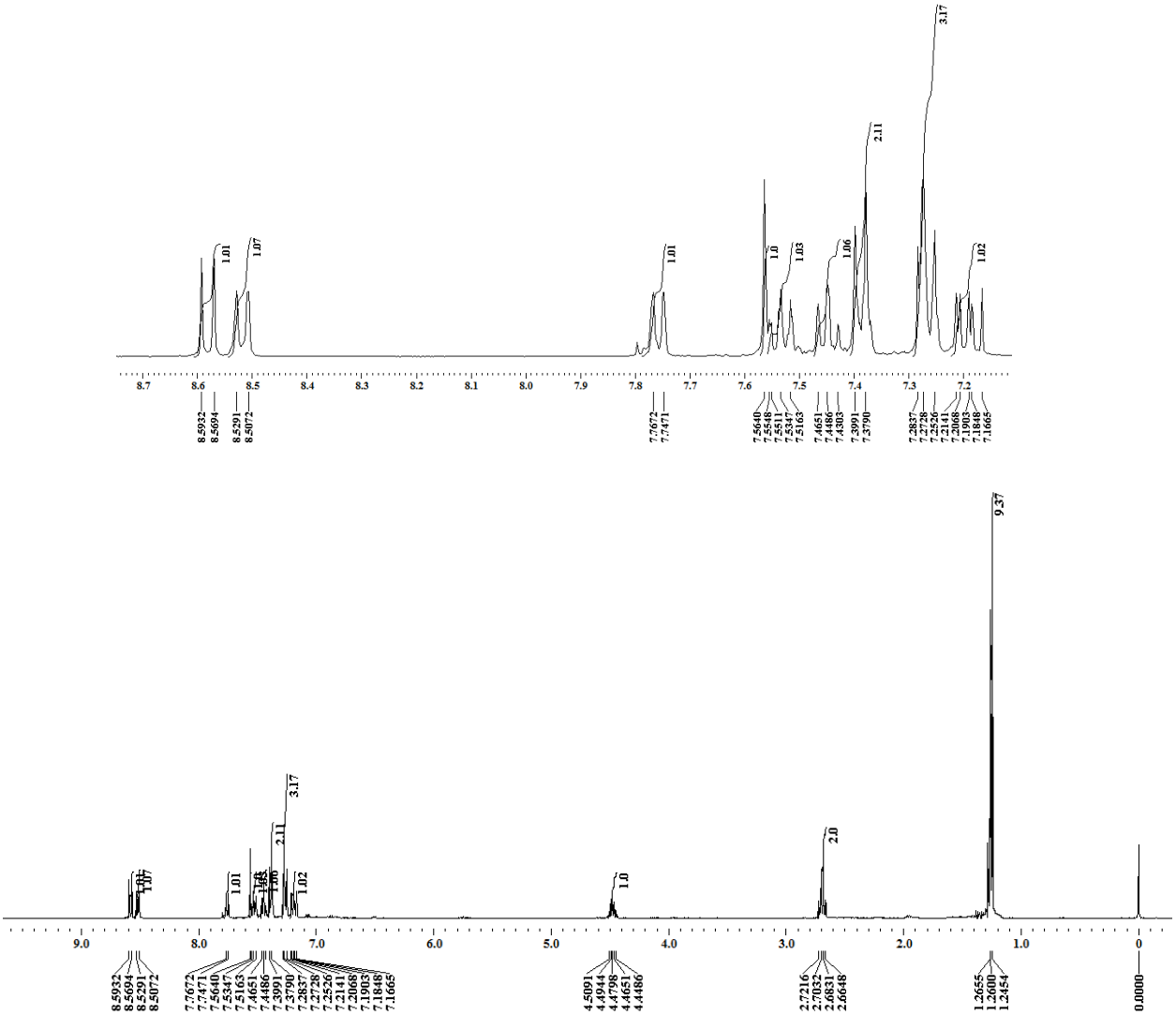

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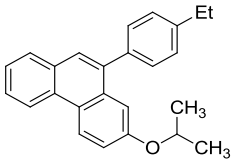
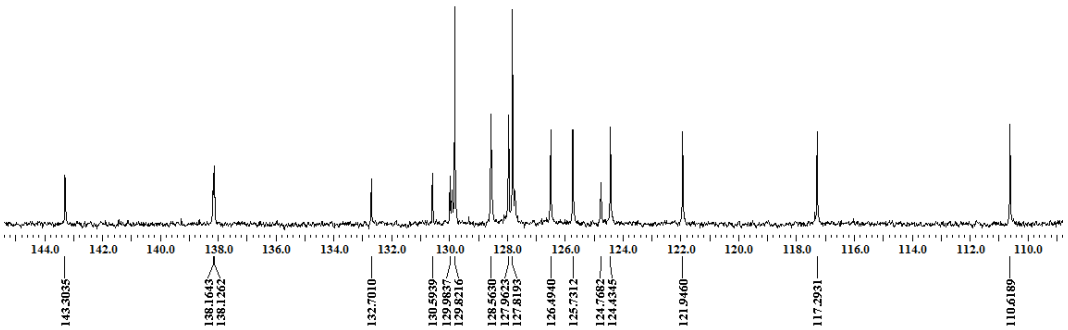
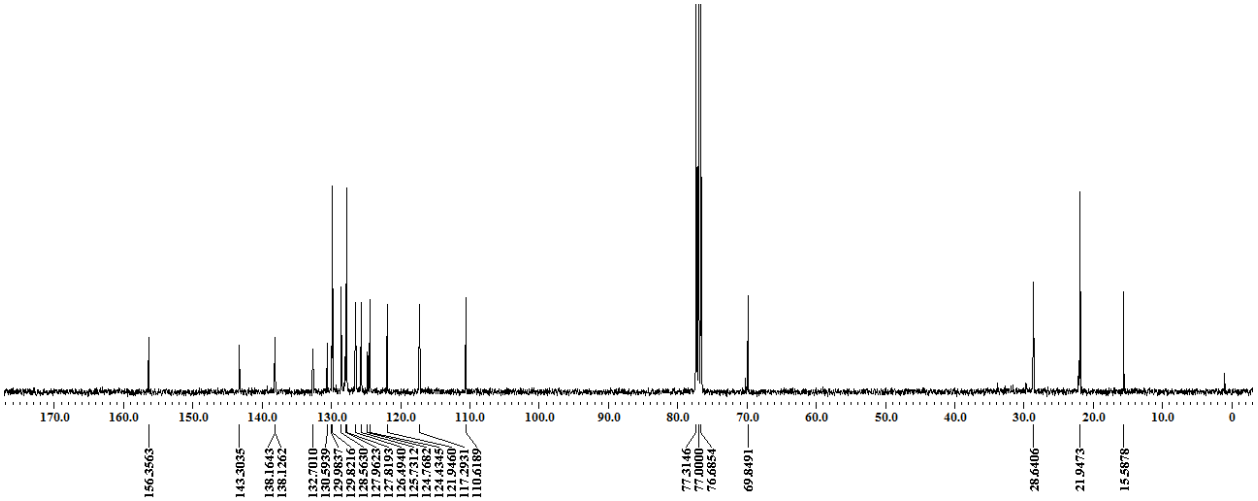
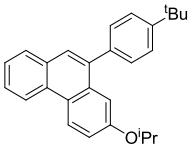


10-(4-Ethylphenyl)-2-isopropoxyphenanthrene (2j)

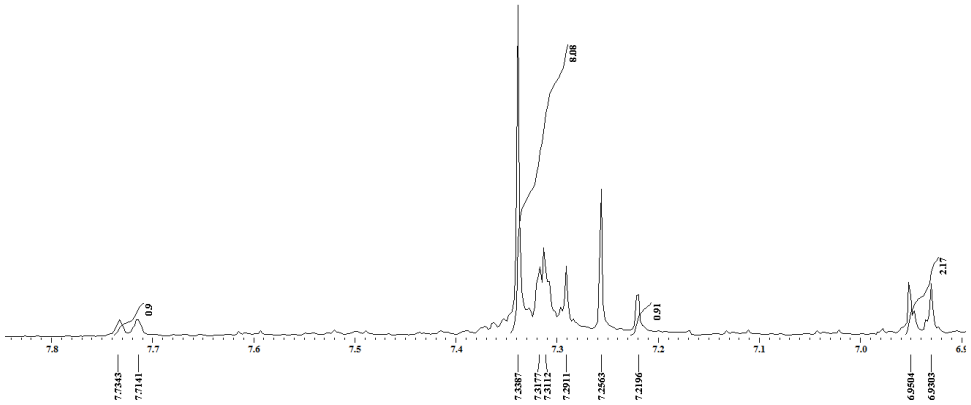


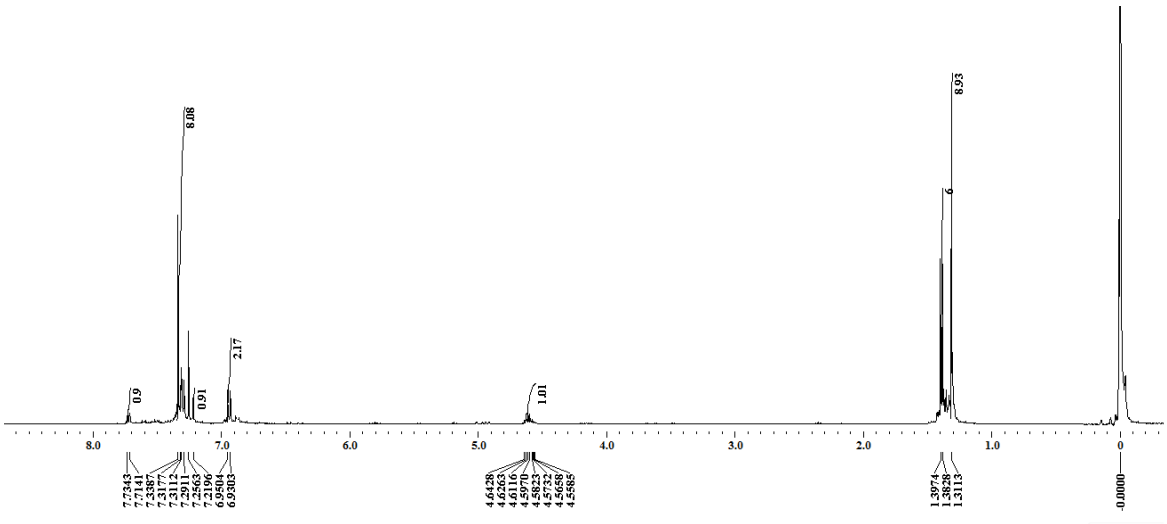


^{1}H NMR

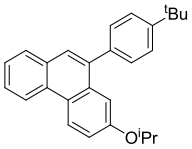


10-(4-*tert*-Butyl-phenyl)-2-propoxy-phenanthrene (2k)

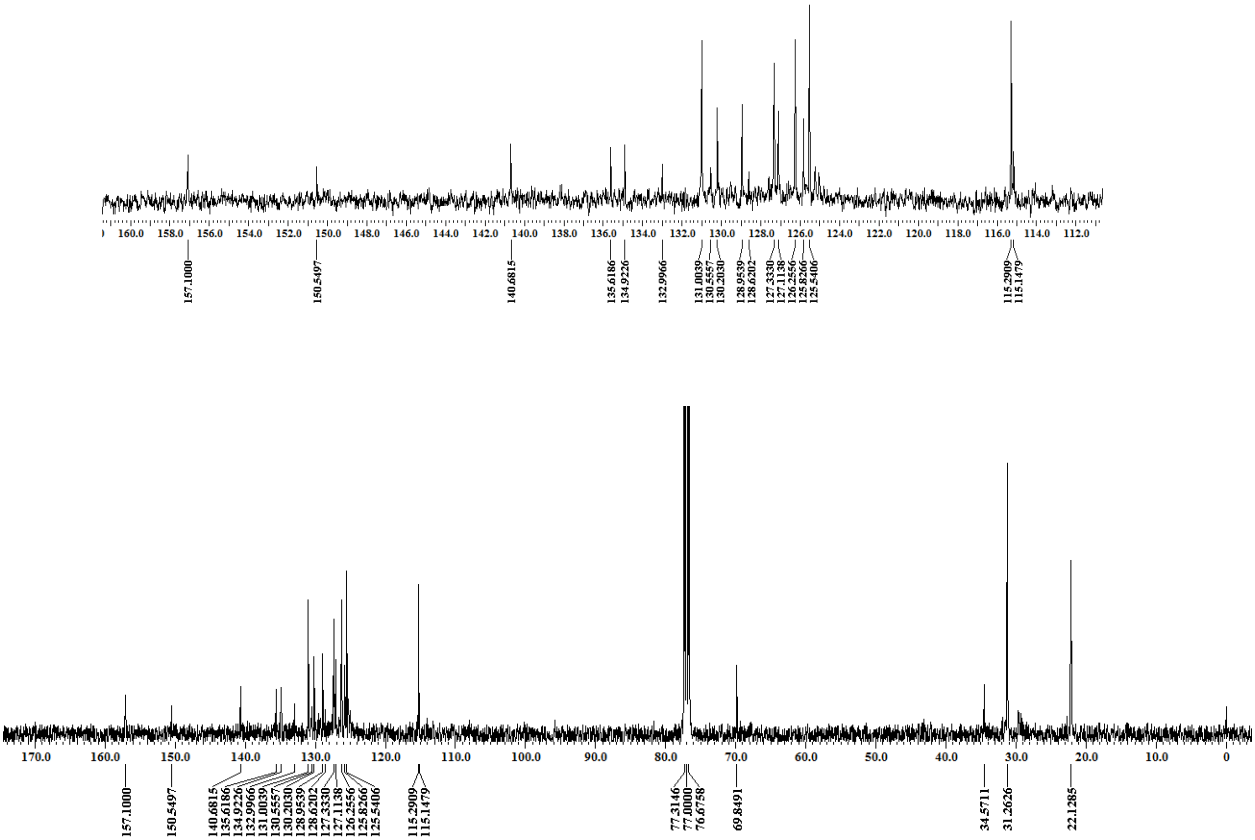




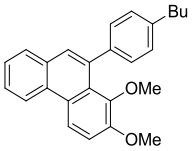
^{13}C NMR



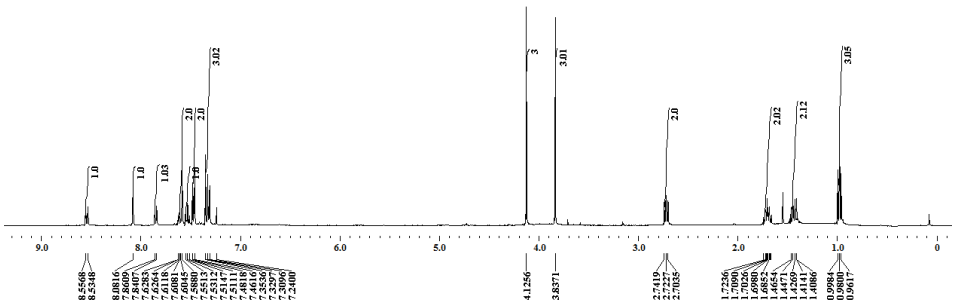
10-(4-*tert*-Butyl-phenyl)-2-propoxy-phenanthrene (2k)

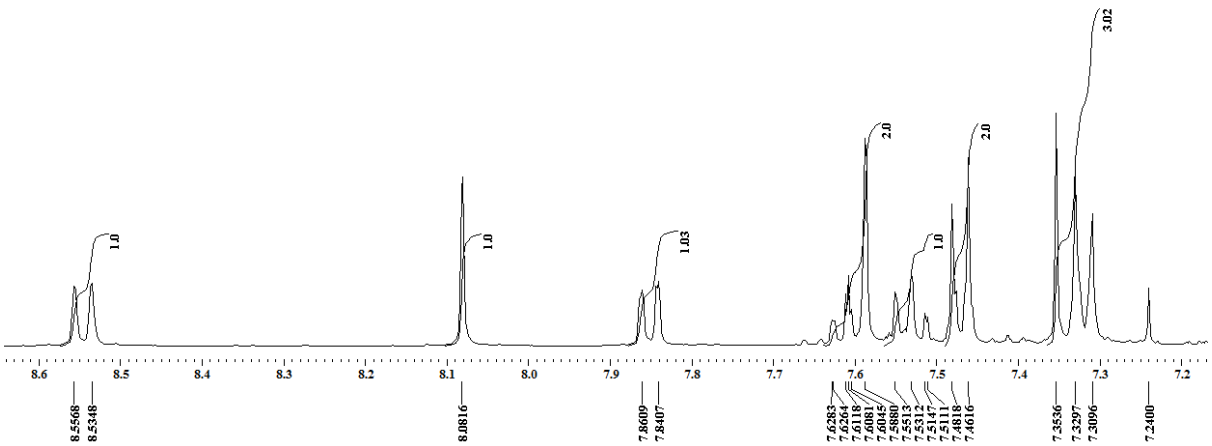


^{1}H NMR

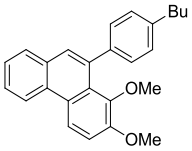


10-(4-butylphenyl)-1,2-dimethoxyphenanthrene (2l)

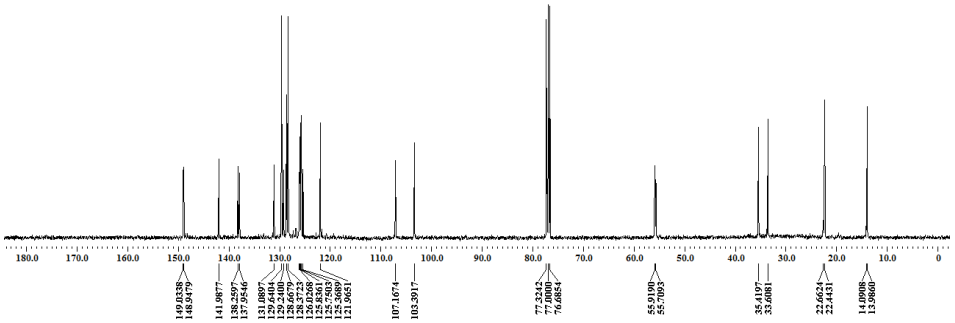


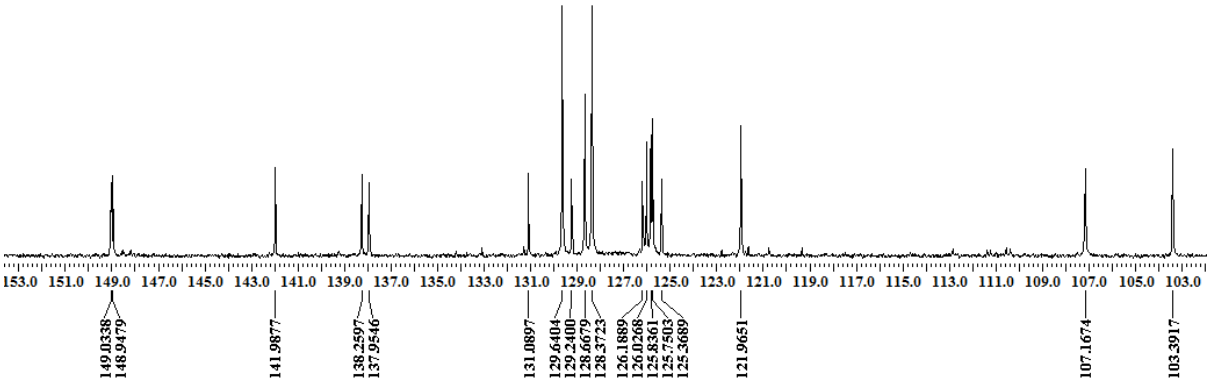


^{13}C NMR

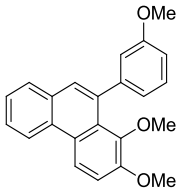


10-(4-butylphenyl)-1,2-dimethoxyphenanthrene (2l)

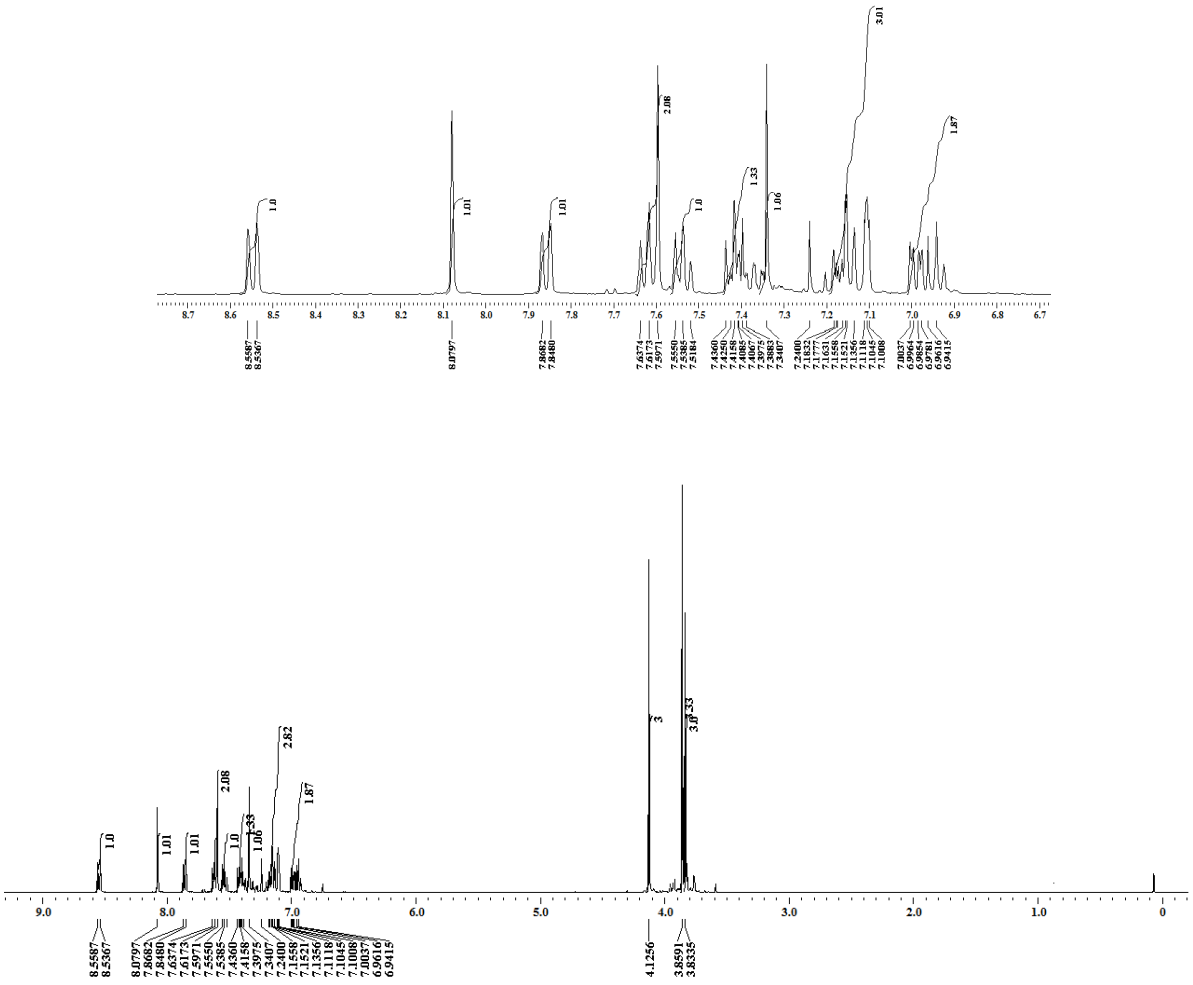




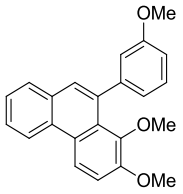
^{1}H NMR



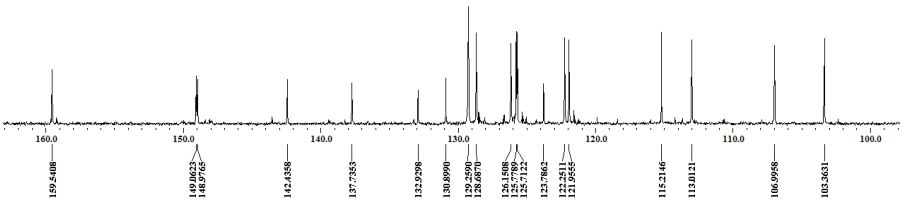
1,2-dimethoxy-10-(3-methoxyphenyl)phenanthrene (2m)

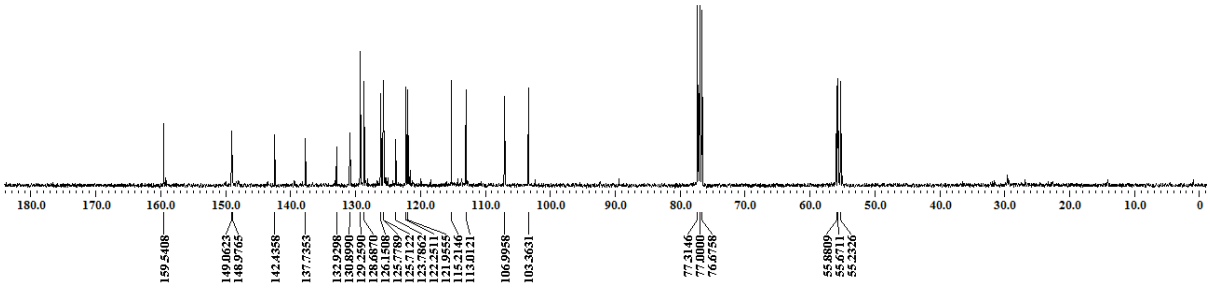


^{13}C NMR

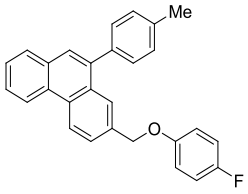


1,2-dimethoxy-10-(3-methoxyphenyl)phenanthrene (2m)

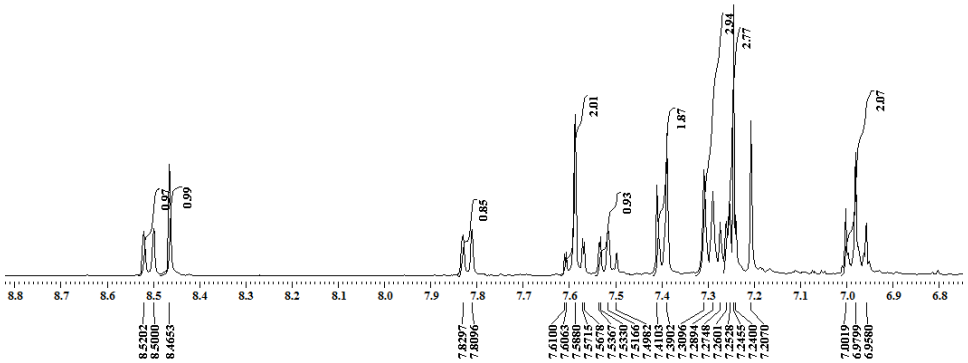


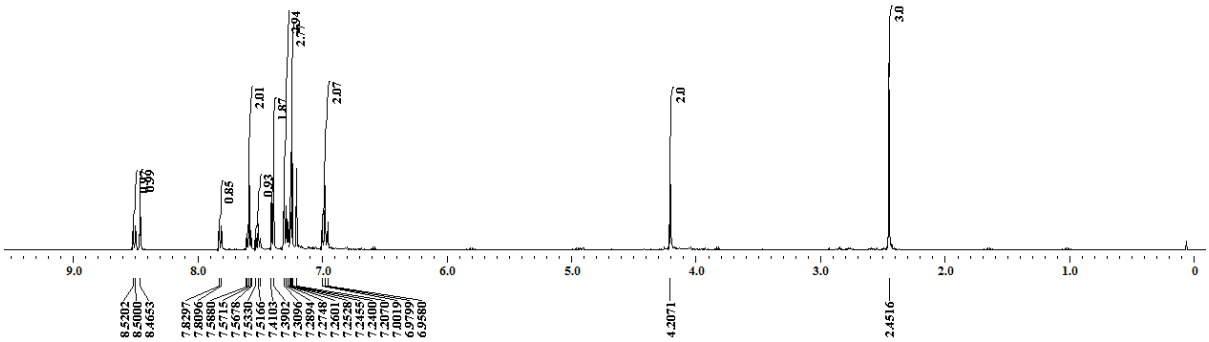


^{1}H NMR

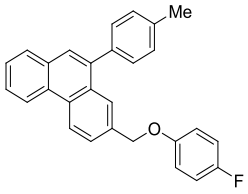


2-(4-Fluoro-phenoxymethyl)-10-*p*-tolyl-phenanthrene (2n)

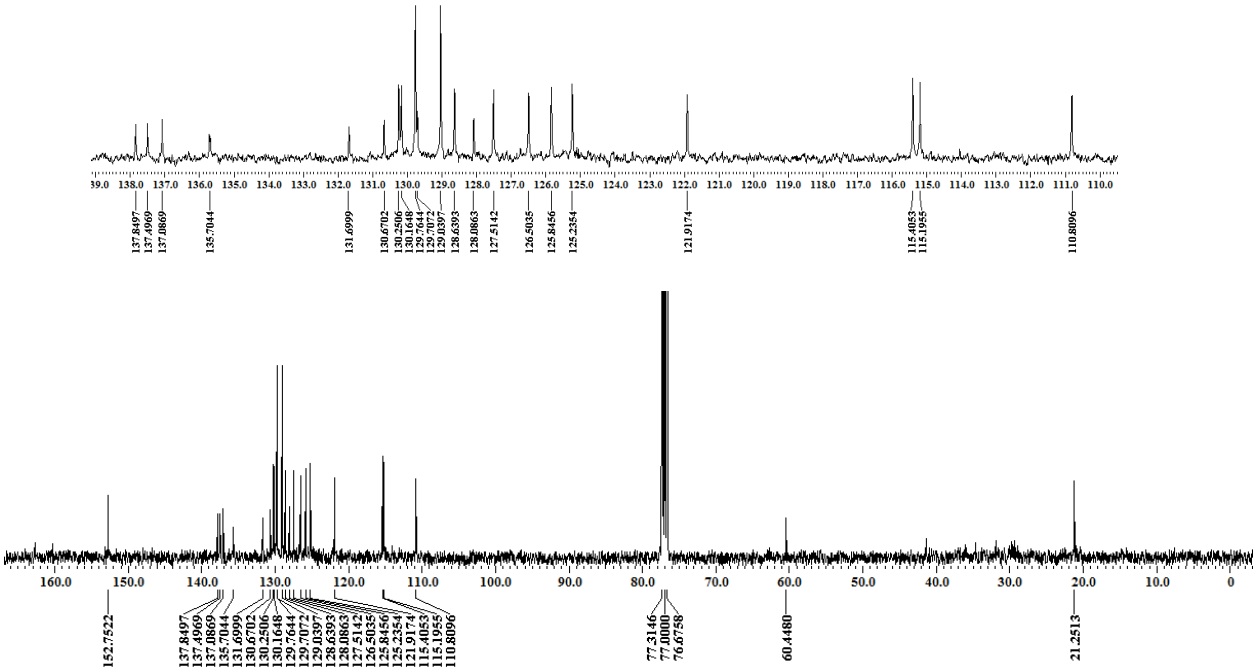




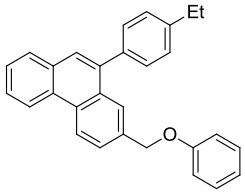
^{13}C NMR



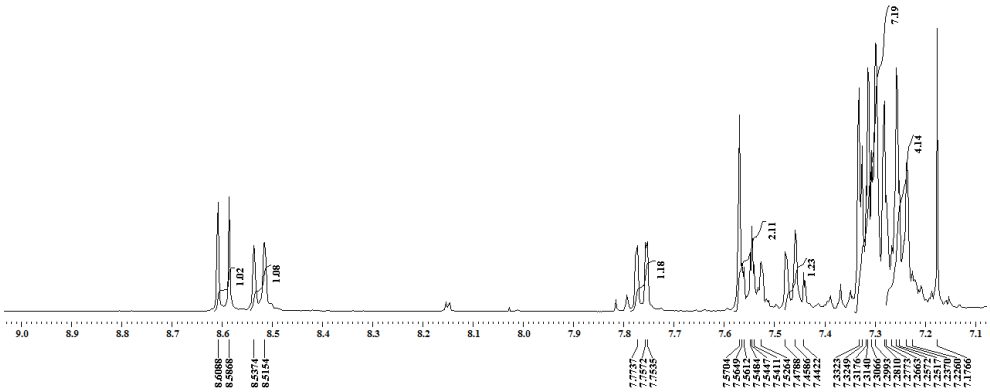
2-(4-Fluoro-phenoxymethyl)-10-*p*-tolyl-phenanthrene (2n)

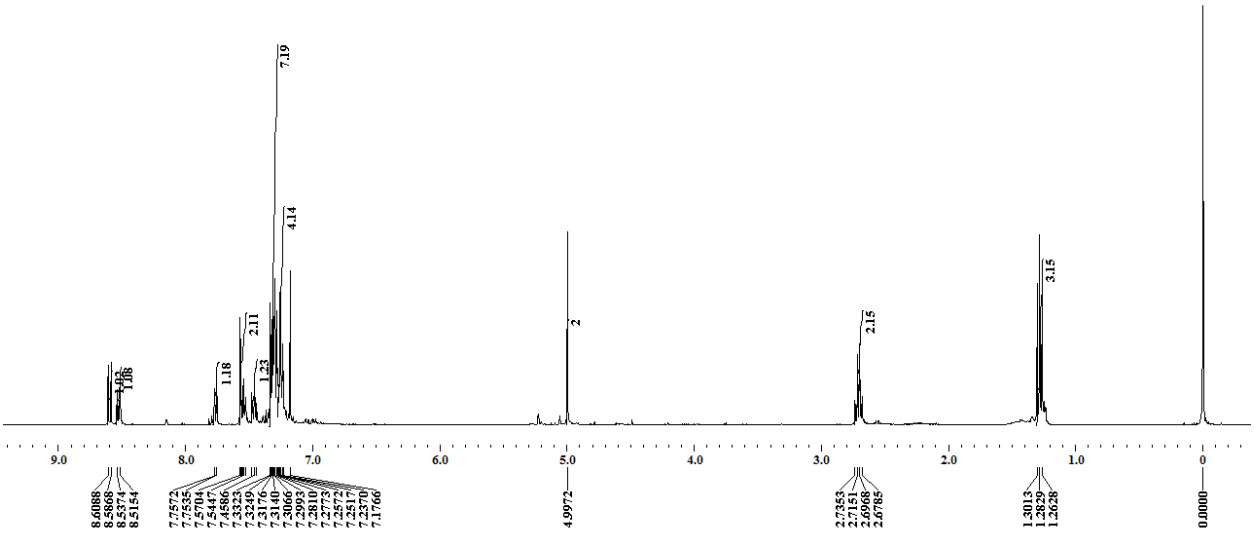


^{1}H NMR

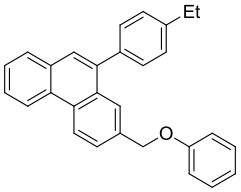


10-(4-Ethylphenyl)-2-(phenoxymethyl)phenanthrene (2o)

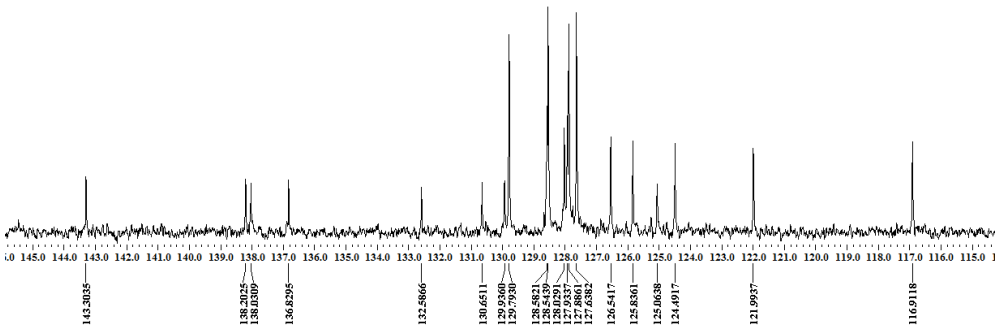


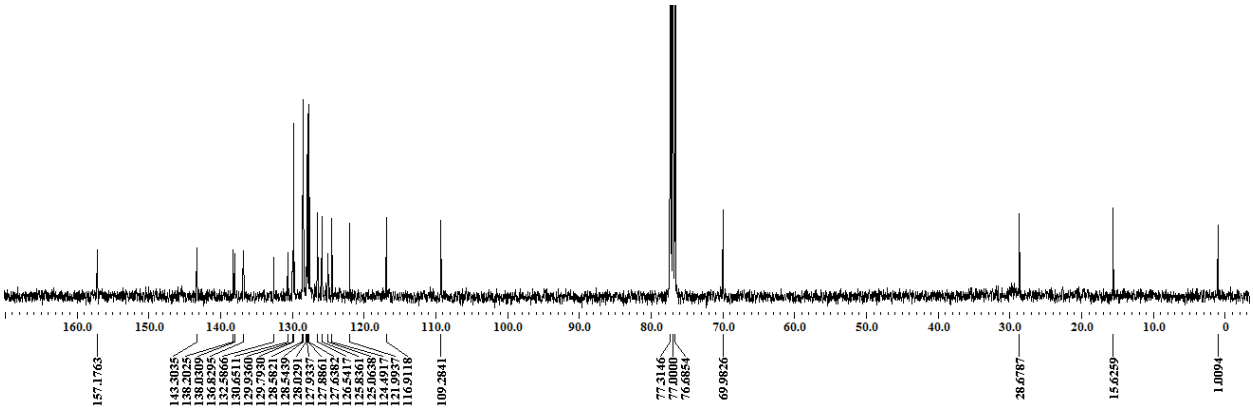


^{13}C NMR

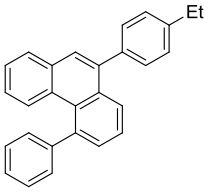


10-(4-Ethylphenyl)-2-(phenoxymethyl)phenanthrene (2o)

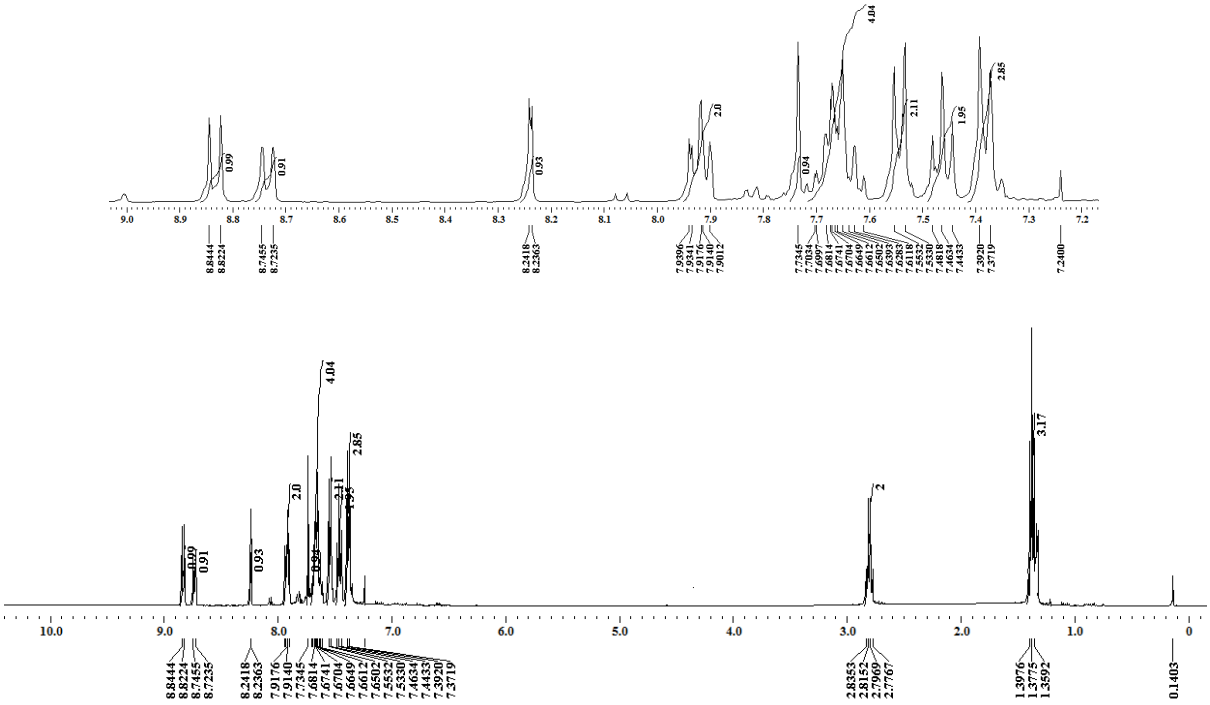




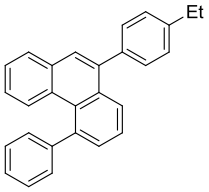
^{1}H NMR



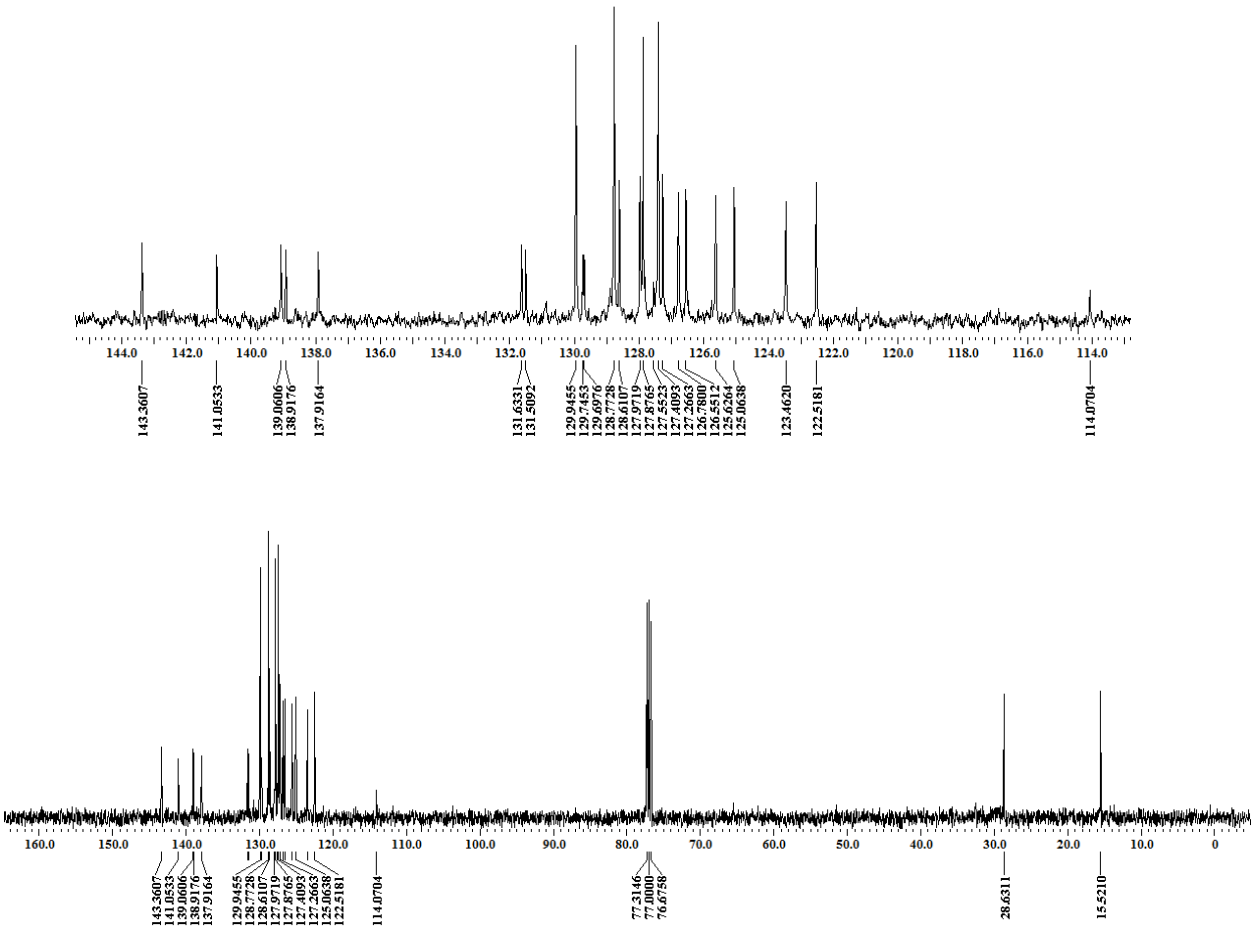
10-(4-Ethylphenyl)-4-phenylphenanthrene (2p)



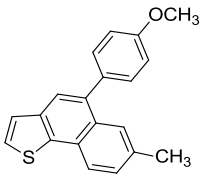
^{13}C NMR



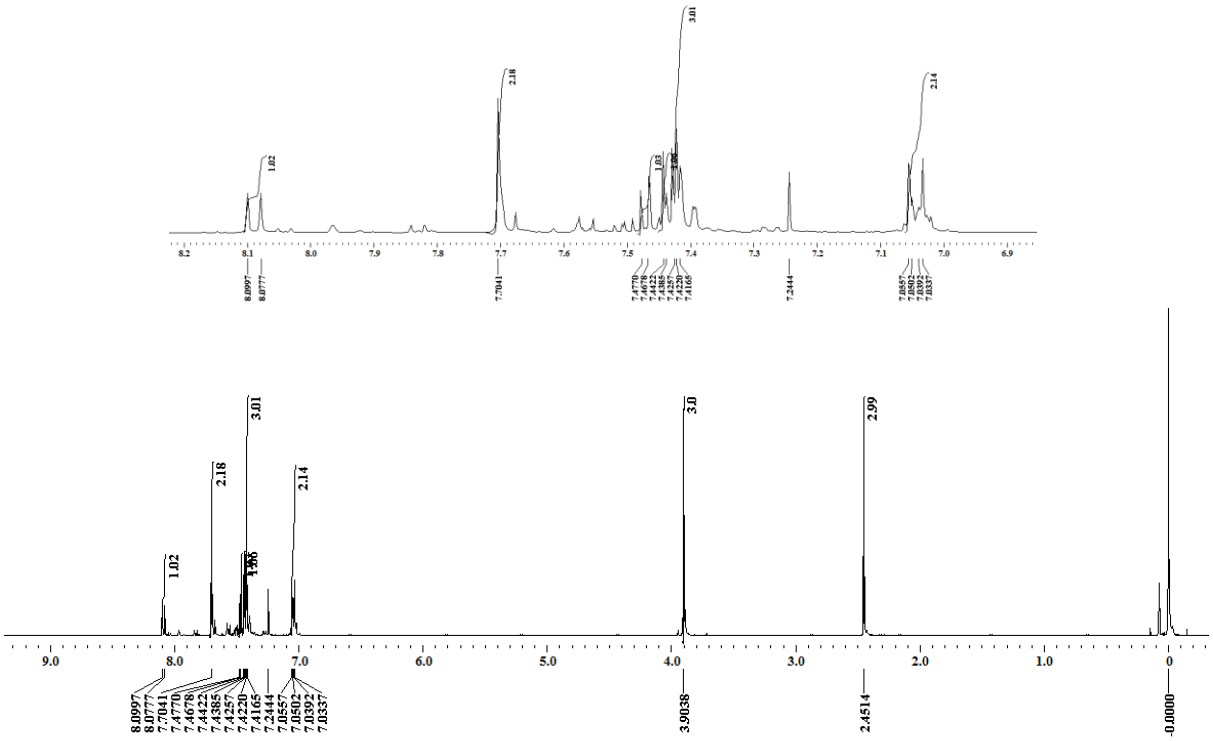
10-(4-Ethylphenyl)-4-phenylphenanthrene (2p)



^{1}H NMR



5-(4-Methoxyphenyl)-7-methylnaphtho[1,2-*b*]thiophene (4a)



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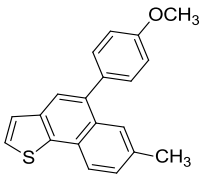
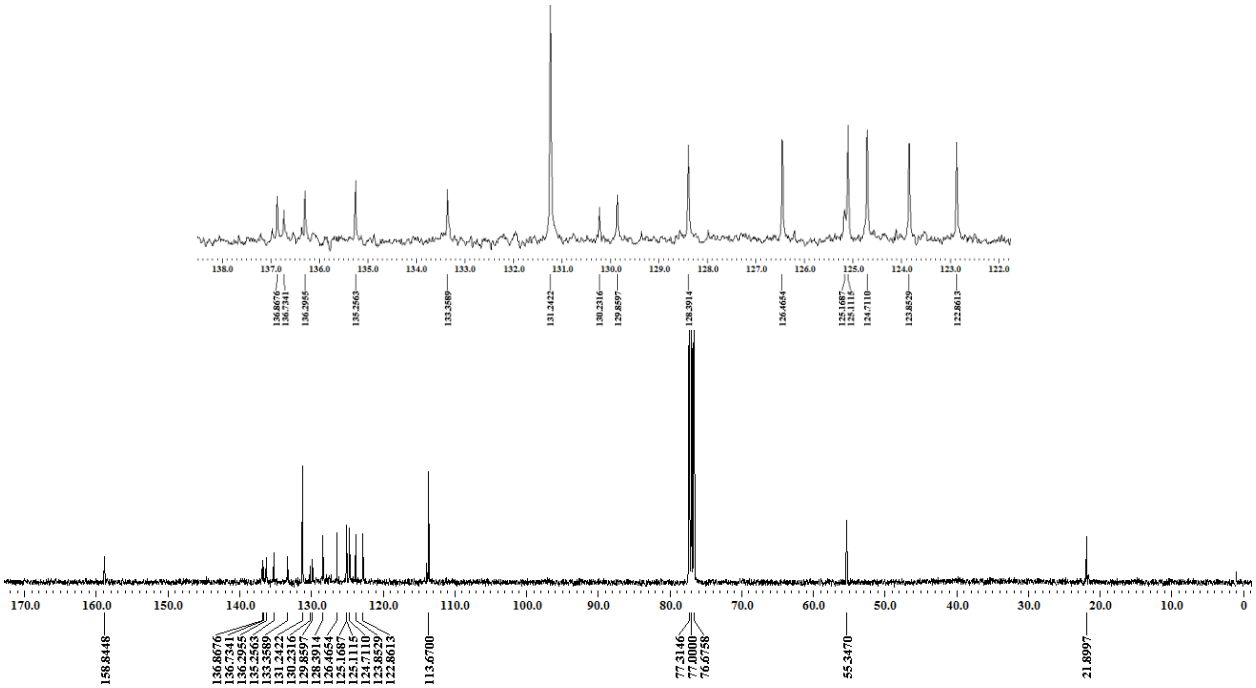
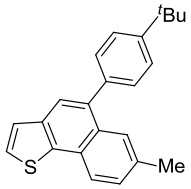


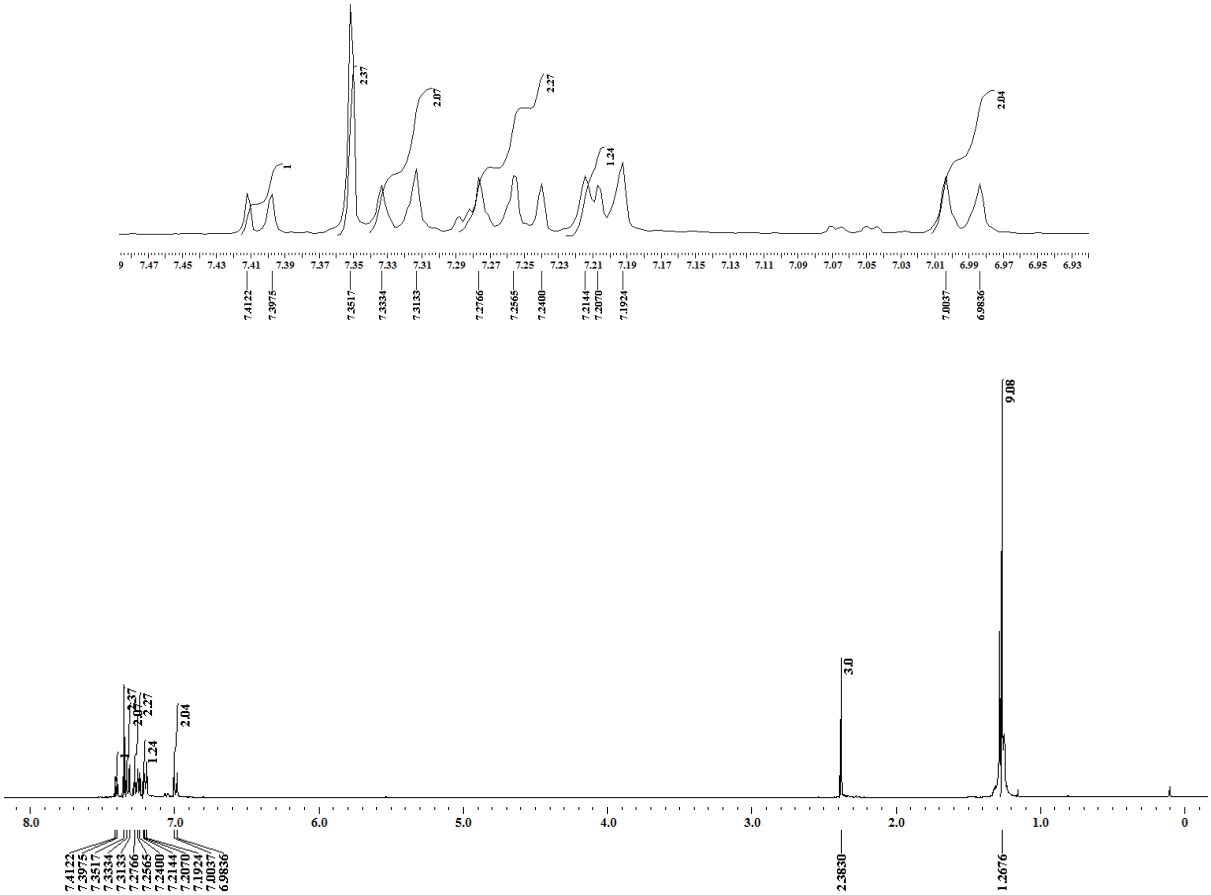
5-(4-Methoxyphenyl)-7-methylnaphtho[1,2-*b*]thiophene (4a)



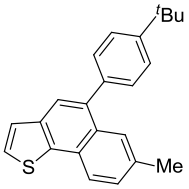
^{1}H NMR



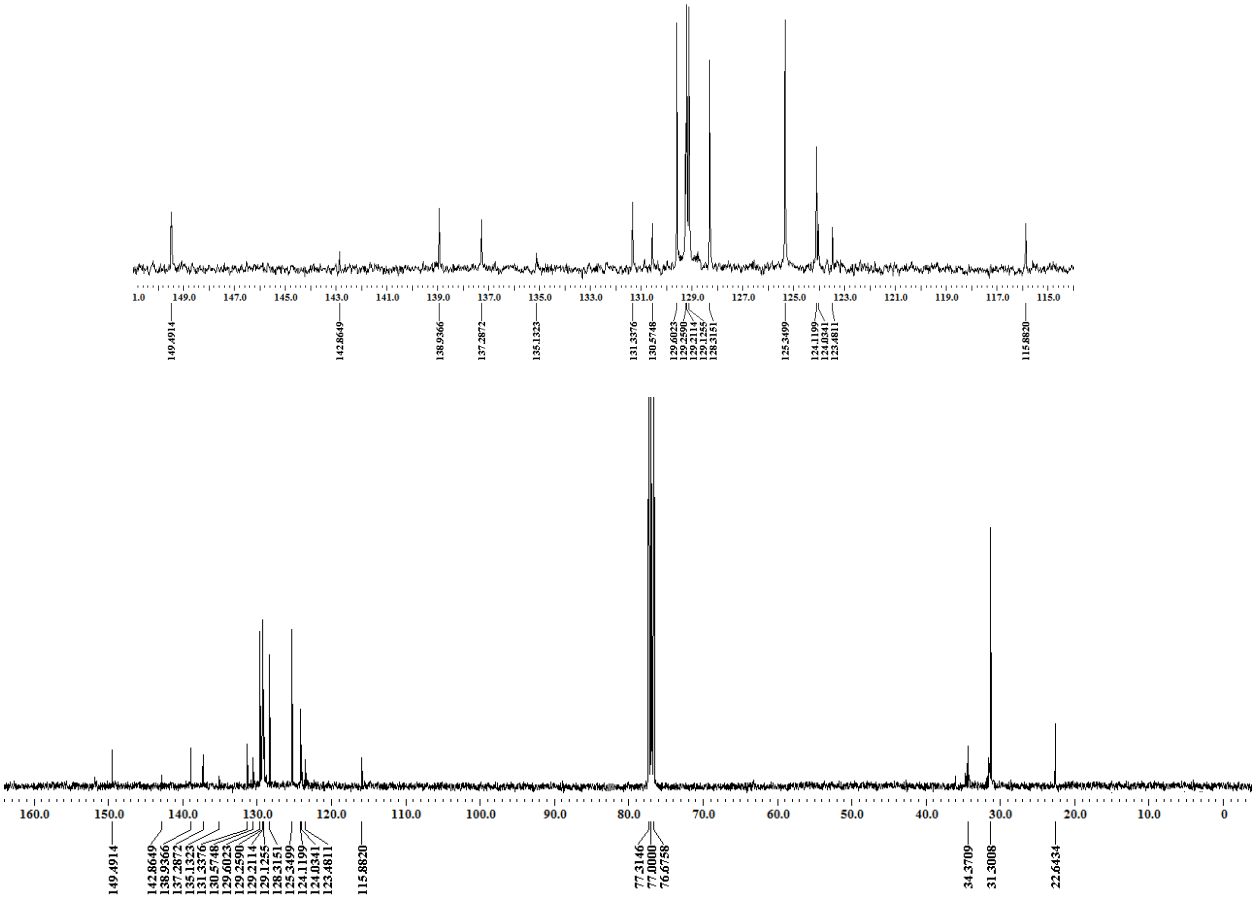
5-(4-(Tert-butyl)phenyl)-7-methylnaphtho[1,2-*b*]thiophene (4b)



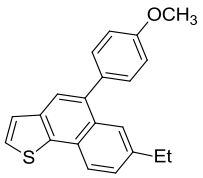
^{13}C NMR



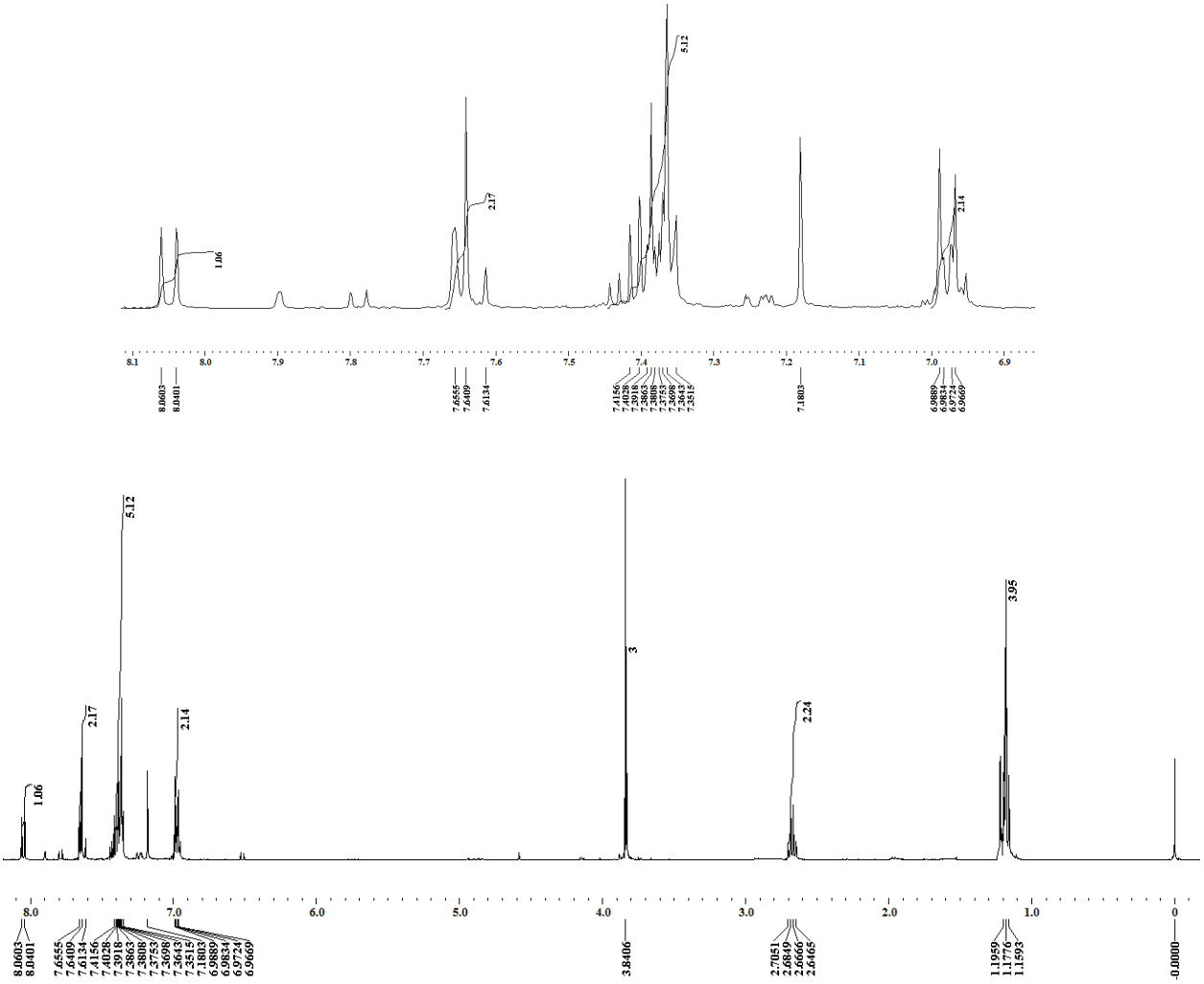
5-(4-(Tert-butyl)phenyl)-7-methylnaphtho[1,2-*b*]thiophene (4b)



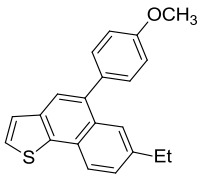
^{1}H NMR



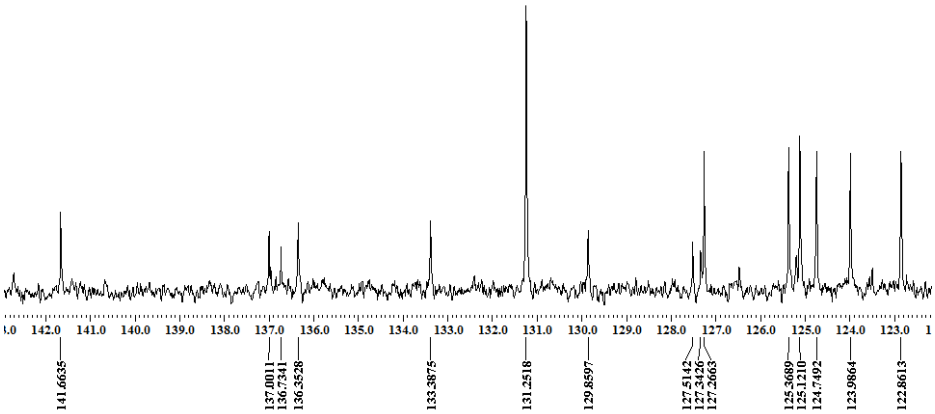
7-Ethyl-5-(4-methoxyphenyl)naphtho[1,2-*b*]thiophene (4c)

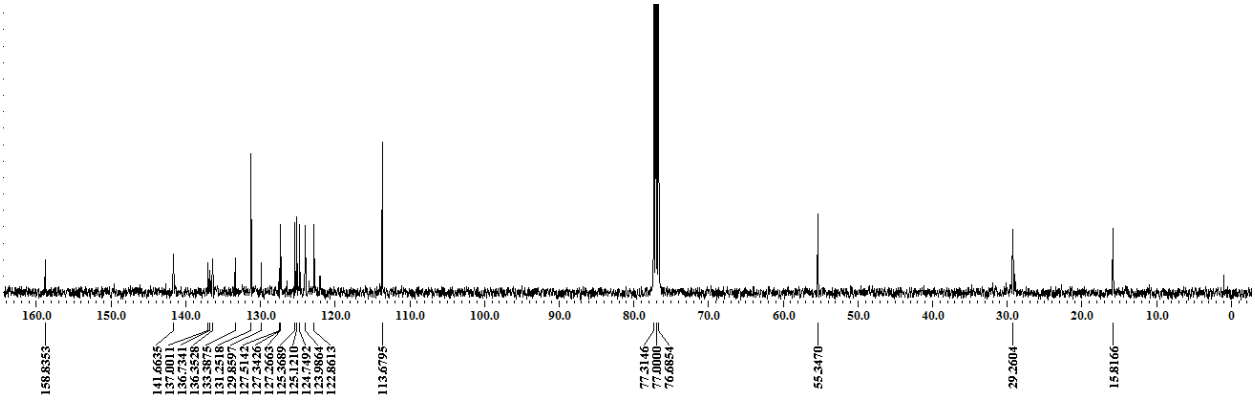


^{13}C NMR

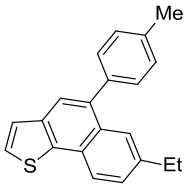


7-Ethyl-5-(4-methoxyphenyl)naphtho[1,2-*b*]thiophene (4c)

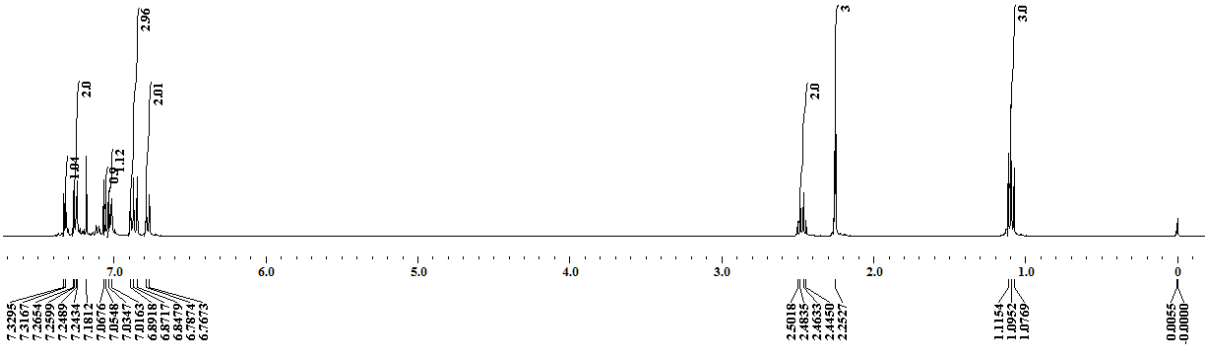




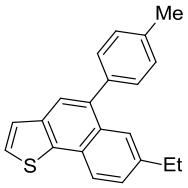
^{1}H NMR



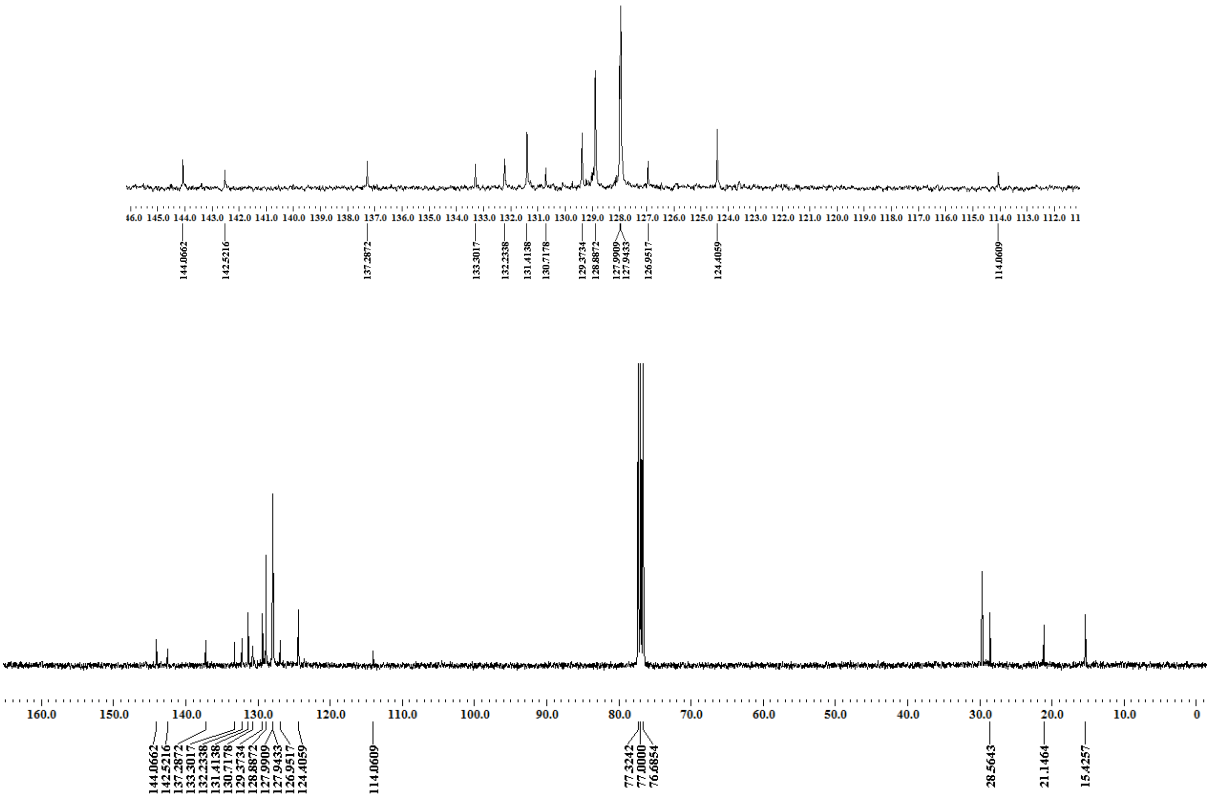
7-Ethyl-5-(p-tolyl)naphtho[1,2-*b*]thiophene (4d)



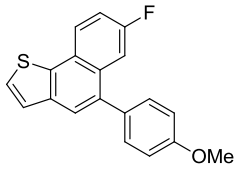
^{13}C NMR



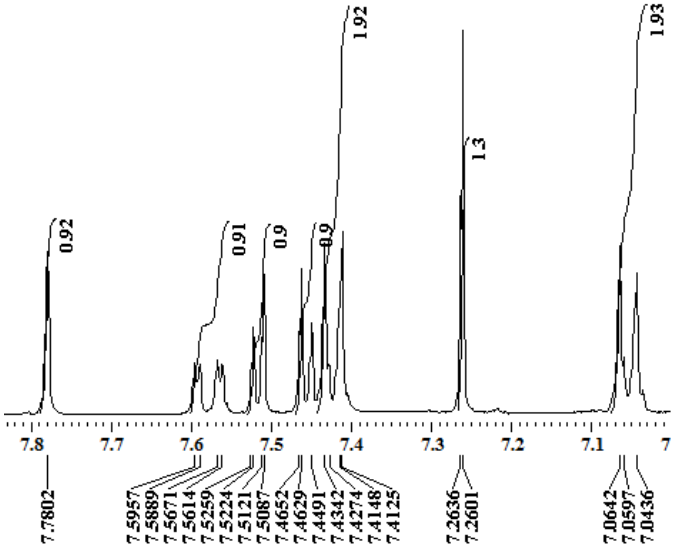
7-Ethyl-5-(*p*-tolyl)naphtho[1,2-*b*]thiophene (4d)

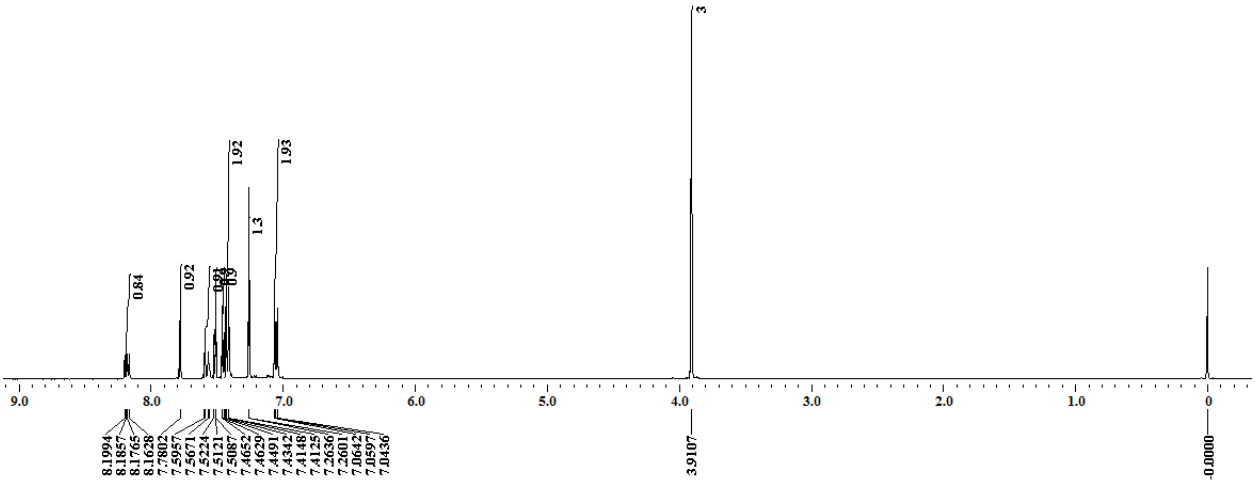


^{1}H NMR

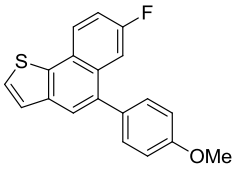


7-Fluoro-5-(4-methoxyphenyl)naphtho[1,2-*b*]thiophene (4e)

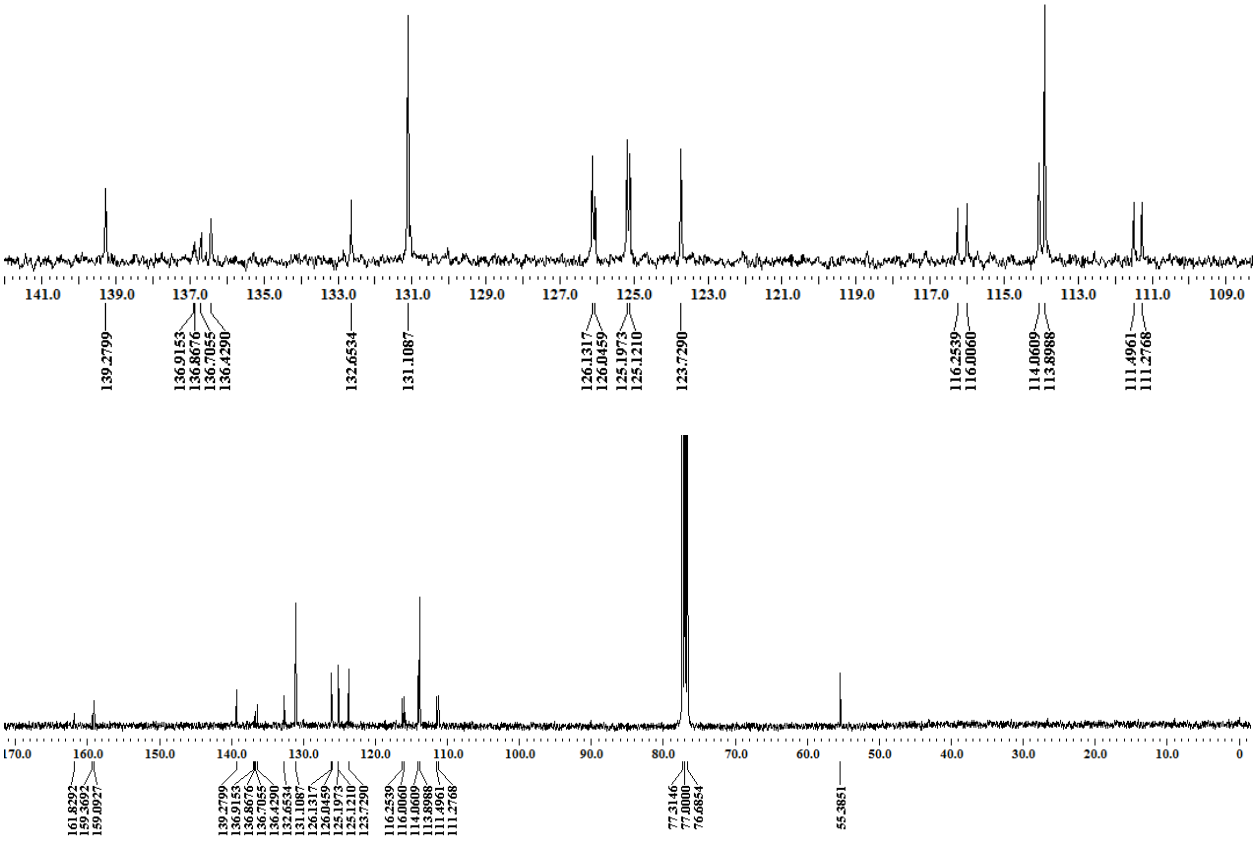




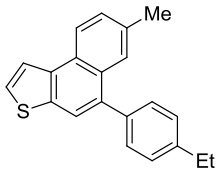
^{13}C NMR



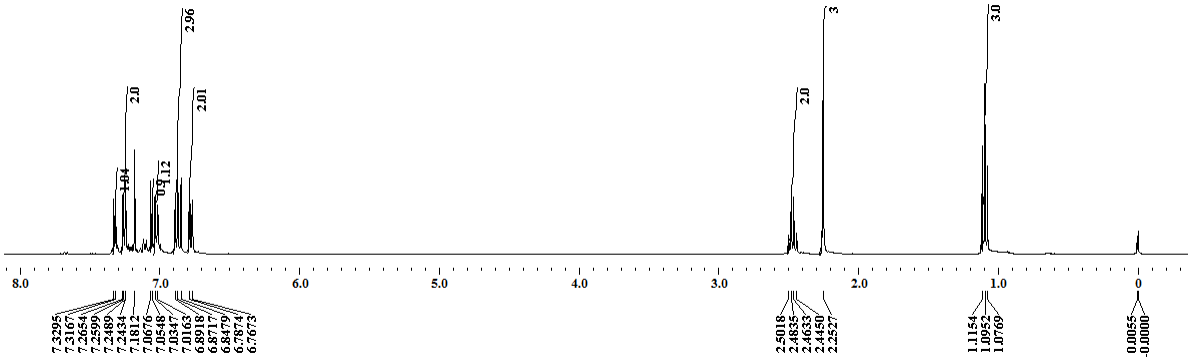
7-Fluoro-5-(4-methoxyphenyl)naphtho[1,2-*b*]thiophene (4e)



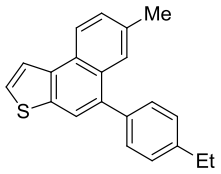
^{1}H NMR



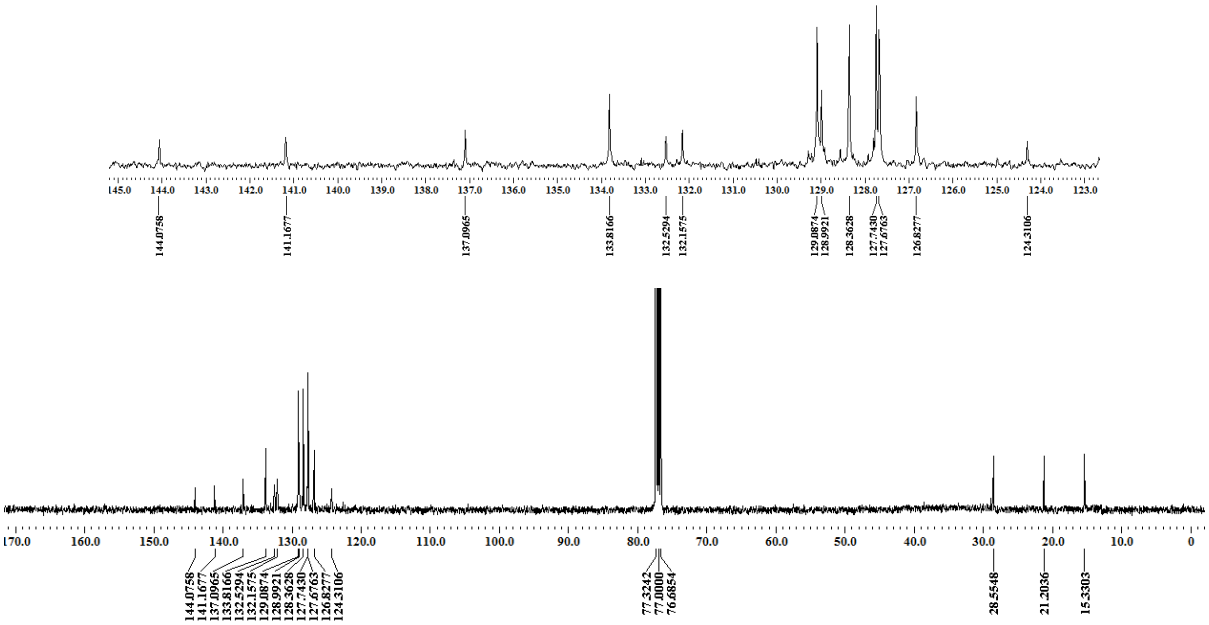
5-(4-Ethylphenyl)-7-methylnaphtho[2,1-*b*]thiophene (6a)



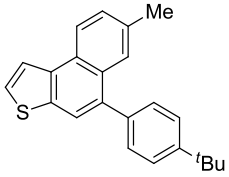
^{13}C NMR



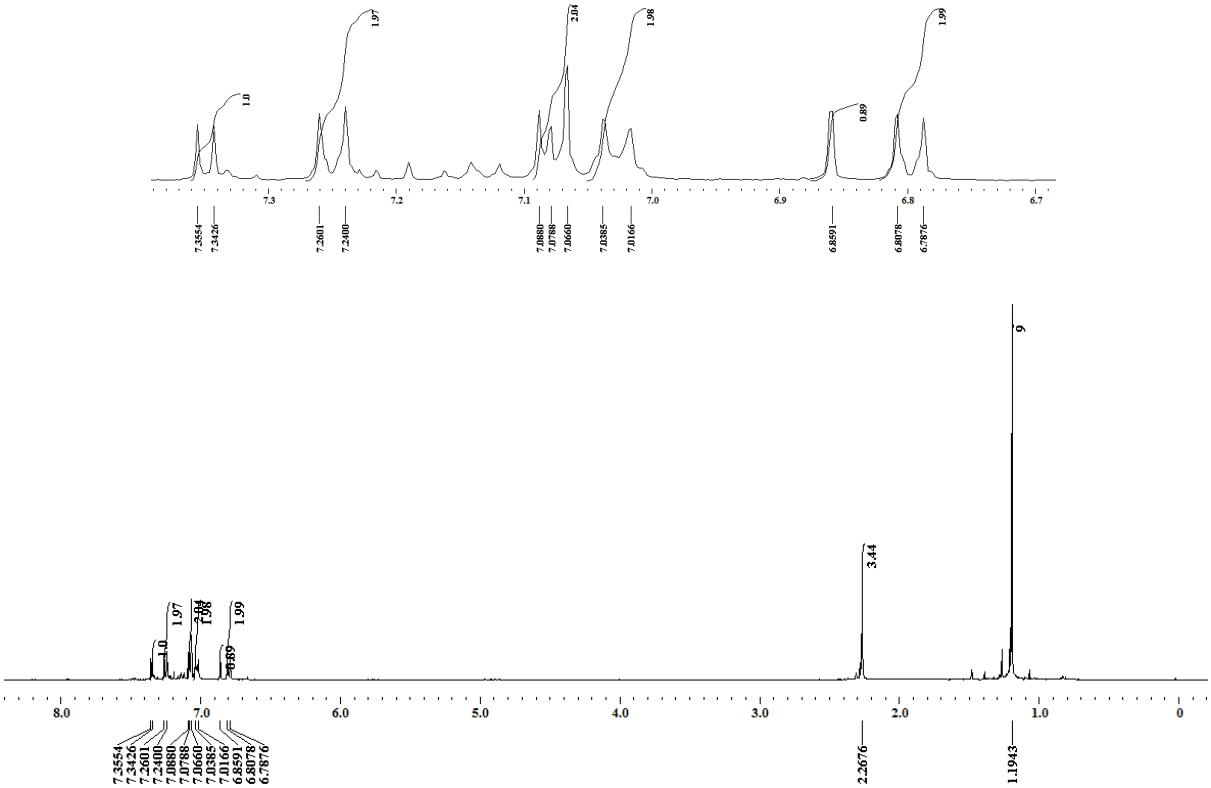
5-(4-Ethylphenyl)-7-methylnaphtho[2,1-*b*]thiophene (6a)



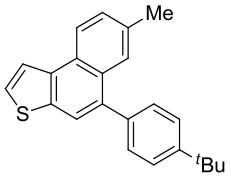
^{1}H NMR



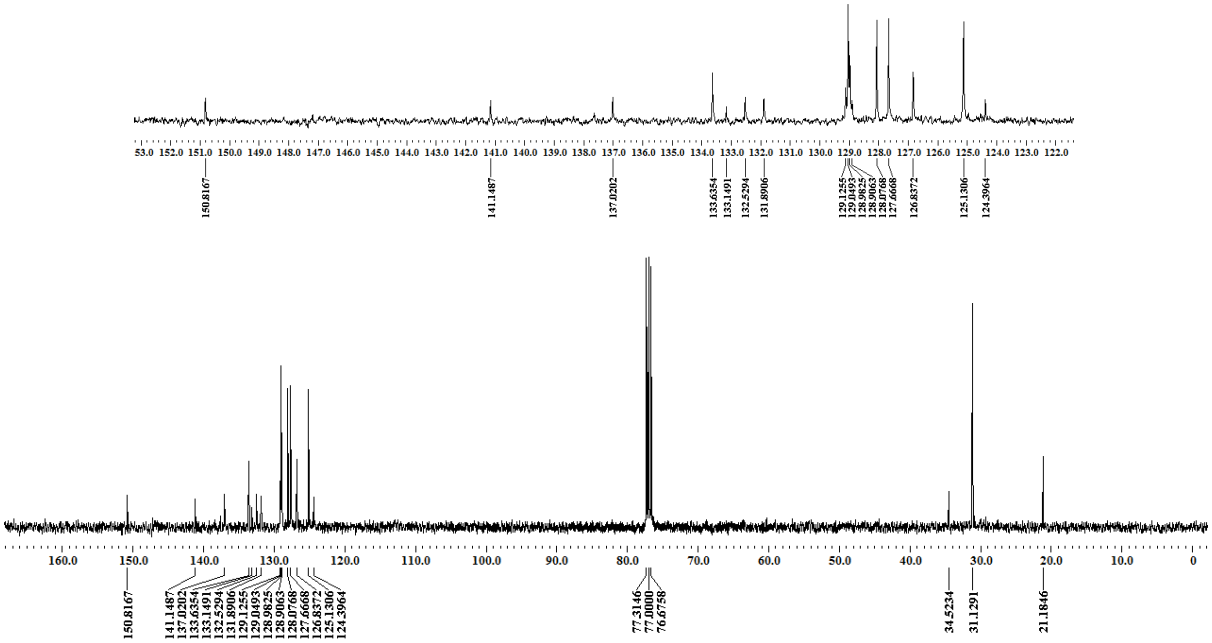
5-(4-(Tert-butyl)phenyl)-7-methylnaphtho[2,1-*b*]thiophene (6b)



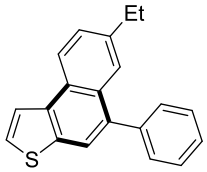
^{13}C NMR



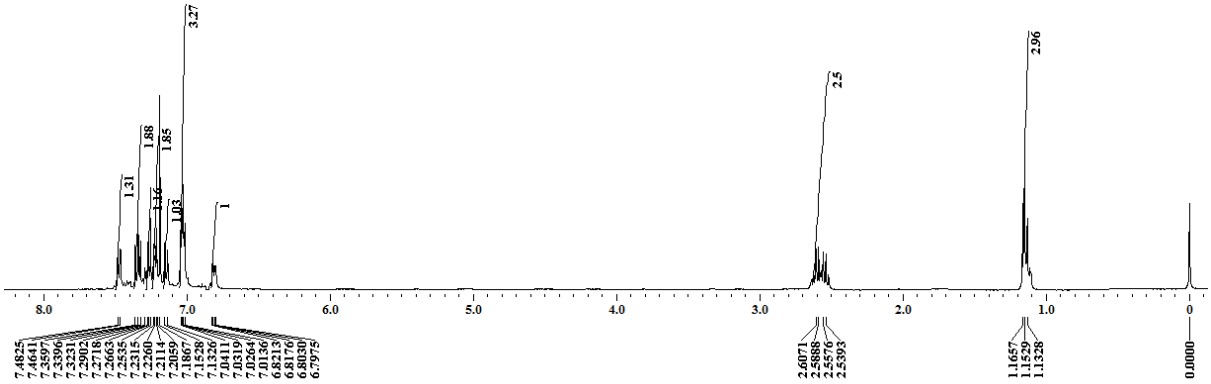
5-(4-(Tert-butyl)phenyl)-7-methylnaphtho[2,1-*b*]thiophene (6b)



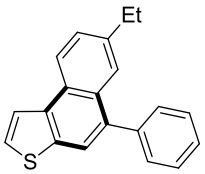
^{1}H NMR



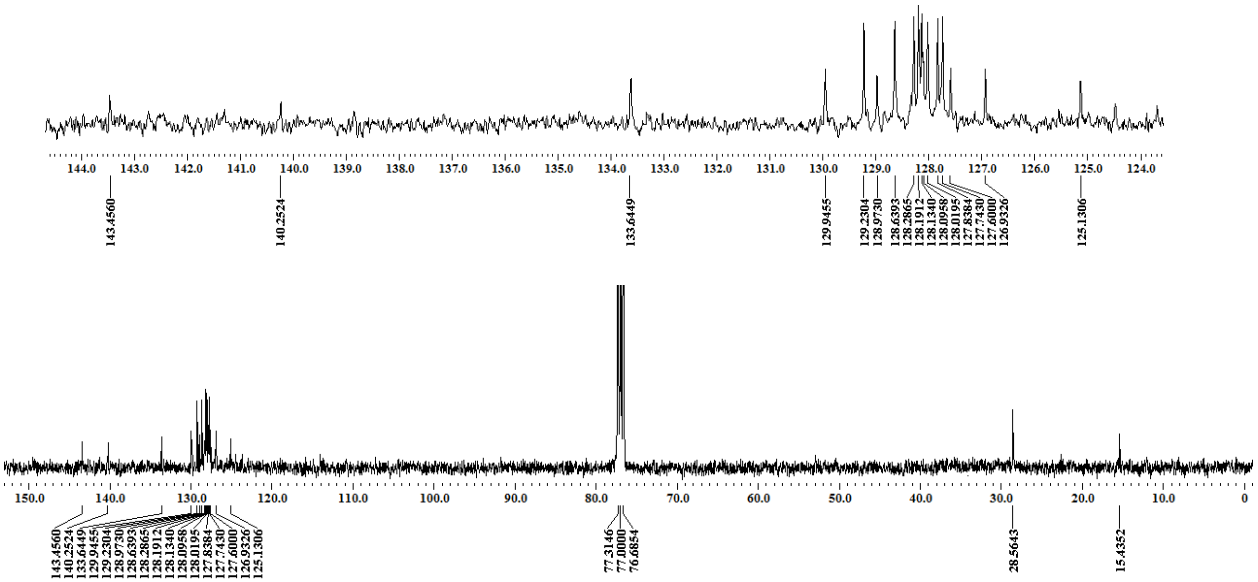
7-Ethyl-5-phenylnaphtho[2,1-*b*]thiophene (6c)



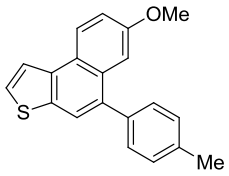
^{13}C NMR



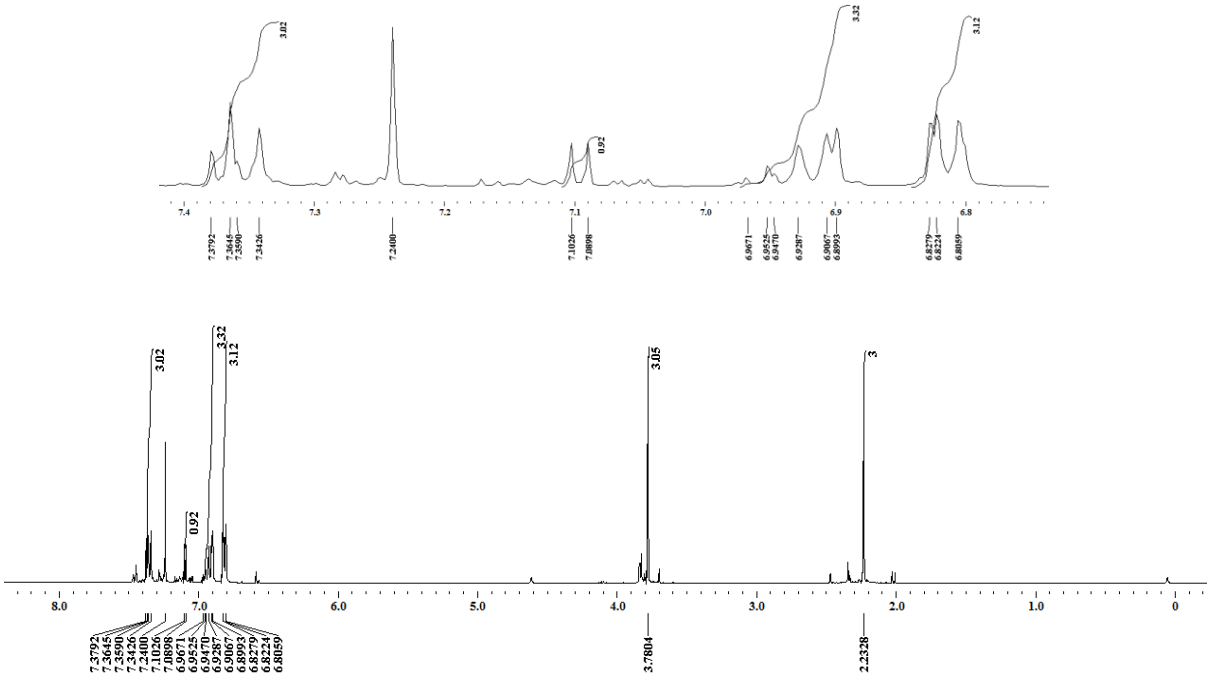
7-Ethyl-5-phenylnaphtho[2,1-*b*]thiophene (6c)



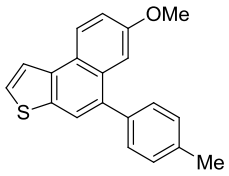
^{1}H NMR



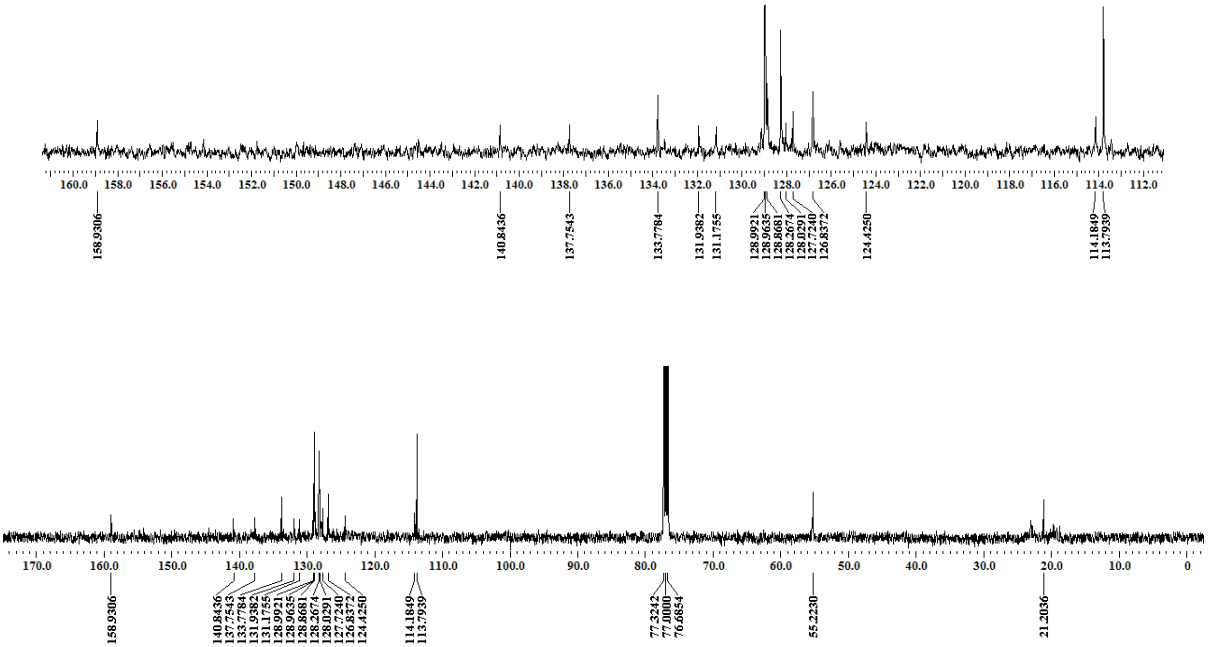
7-Methoxy-5-(*p*-tolyl)naphtho[2,1-*b*]thiophene (6d)



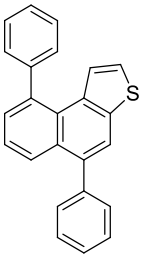
^{13}C NMR



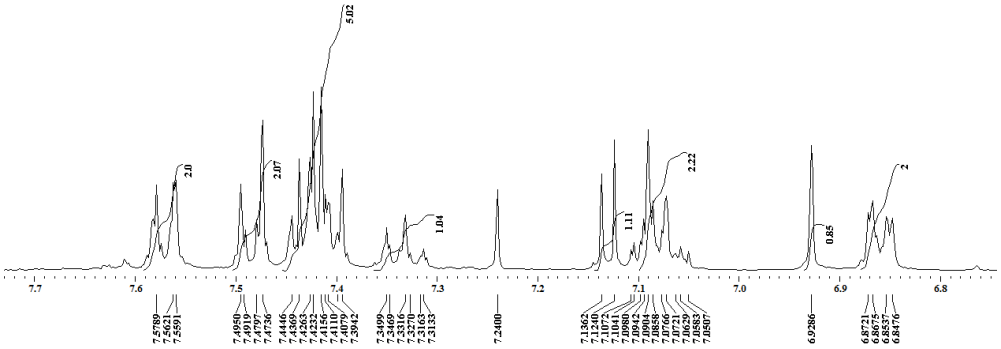
7-Methoxy-5-(*p*-tolyl)naphtho[2,1-*b*]thiophene (6d)

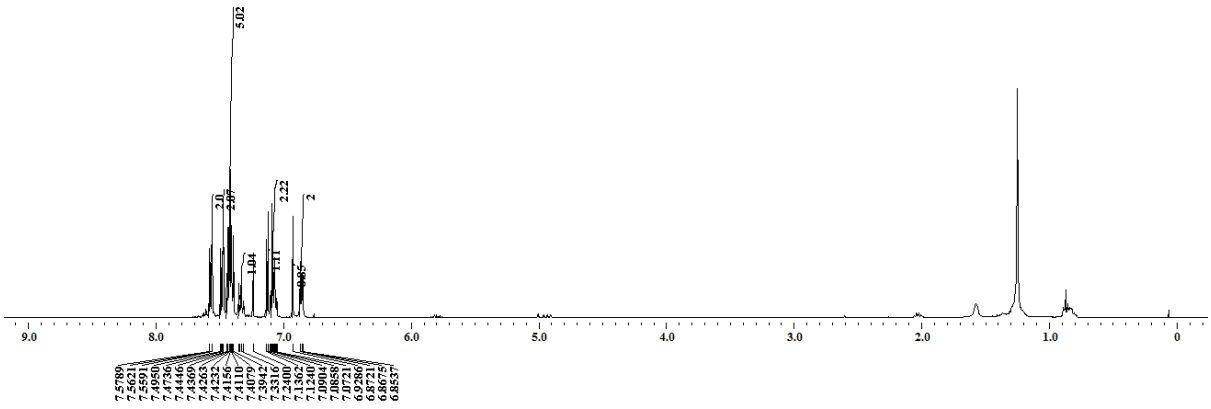


^{1}H NMR

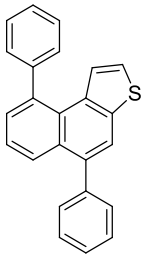


5,9-Diphenylnaphtho[2,1-*b*]thiophene (6e)





^{13}C NMR



5,9-Diphenylnaphtho[2,1-*b*]thiophene (6e)